



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 07:24 AM BST

PDB ID : 4V5F
Title : The structure of the ribosome with elongation factor G trapped in the post-translocational state
Authors : Gao, Y.-G.; Selmer, M.; Dunham, C.M.; Weixlbaumer, A.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2009-09-01
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

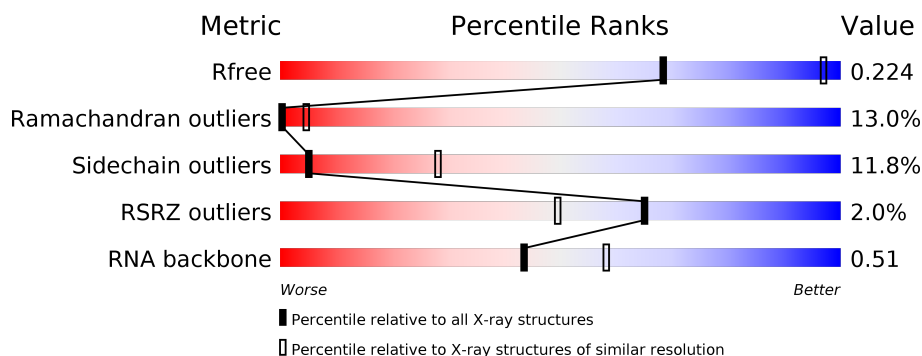
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

















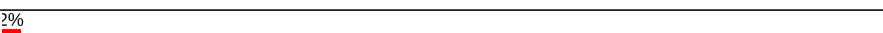




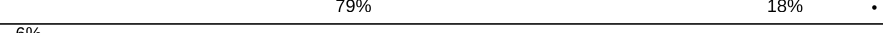





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>••</div> </div> </div>
1	CA	1522	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>••</div> </div> </div>
2	AB	256	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>•</div> <div>8%</div> </div> </div>
2	CB	256	<div> <div></div> <div> <div>70%</div> <div>19%</div> <div>•</div> <div>8%</div> </div> </div>
3	AC	239	<div> <div></div> <div> <div>72%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>
3	CC	239	<div> <div></div> <div> <div>72%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>






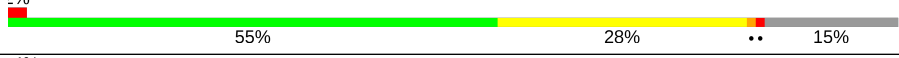

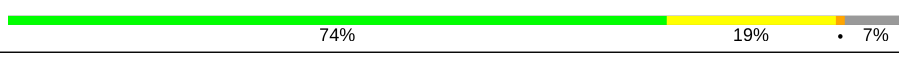



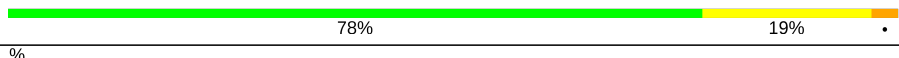








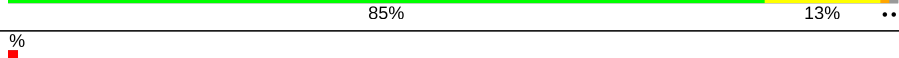
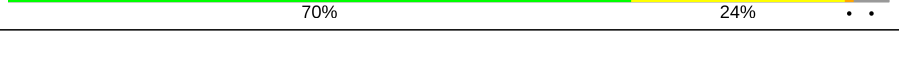

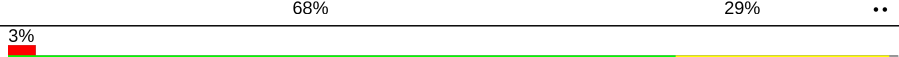

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Mol	Chain	Length	Quality of chain
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	

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Mol	Chain	Length	Quality of chain
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	AW	77	
22	CV	77	
22	CW	77	
23	AX	25	
23	CX	25	
24	AY	691	
24	CY	691	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	
27	B2	72	
27	D2	72	

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Mol	Chain	Length	Quality of chain
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2915	
35	DA	2915	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	
39	DE	206	
40	BF	210	

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Mol	Chain	Length	Quality of chain
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BJ	173	
43	DJ	173	
44	BK	147	
44	DK	147	
45	BL	125	
45	BM	125	
45	Bl	125	
45	Bm	125	
45	DL	125	
45	DM	125	
45	Dl	125	
45	Dm	125	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	

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Mol	Chain	Length	Quality of chain
50	BR	118	 79% 19% 2% 2%
50	DR	118	 77% 21% 2% 2%
51	BS	112	 63% 25% 2% 12%
51	DS	112	 63% 25% 4% 12%
52	BT	146	 62% 29% 3% 5%
52	DT	146	 61% 31% 3% 5%
53	BU	118	 81% 18% 1% 0%
53	DU	118	 81% 19% 1% 0%
54	BV	101	 73% 25% 2% 0%
54	DV	101	 73% 25% 6% 0%
55	BW	113	 86% 13% 1% 0%
55	DW	113	 87% 12% 1% 0%
56	BX	96	 78% 18% 2% 2%
56	DX	96	 78% 18% 2% 2%
57	BY	110	 64% 32% 2% 2%
57	DY	110	 65% 31% 4% 2%
58	BZ	206	 65% 20% 5% 10%
58	DZ	206	 67% 21% 1% 10%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 311552 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called E-SITE TRNA FMET OR P-SITE TRNA FMET (UN-MODIFIED BASES EXCEPT FOR THYMINE 54).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	11	Total	C	N	O	P	0	0	0
			230	105	41	74	10			
23	CX	11	Total	C	N	O	P	0	0	0
			230	105	41	74	10			

- Molecule 24 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			
24	CY	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
25	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
27	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			
29	D4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
32	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
34	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			
35	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
36	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
37	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
38	DD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
39	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
40	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
41	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	167	Total	C	N	O	S	0	0	1
			1269	803	238	227	1			
42	DH	167	Total	C	N	O	S	0	0	1
			1269	803	238	227	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BJ	170	Total	C	N	O	S	0	0	0
			851	510	170	171				
43	DJ	170	Total	C	N	O	S	0	0	0
			851	510	170	171				

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	140	Total	C	N	O	S	0	0	1
			1026	653	182	186	5			
44	DK	140	Total	C	N	O	S	0	0	1
			1026	653	182	186	5			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BL	102	Total	C	N	O		0	0	1
			506	303	102	101				
45	BM	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Bl	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Bm	30	Total	C	N	O		0	0	1
			146	87	30	29				
45	DL	102	Total	C	N	O		0	0	1
			506	303	102	101				
45	DM	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Dl	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Dm	30	Total	C	N	O		0	0	1
			146	87	30	29				

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
46	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
47	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
48	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
49	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
50	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	0	0	1
			1142	710	235	196			
52	DT	138	Total	C	N	O	0	0	1
			1142	710	235	196			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	BU	117	Total	C	N	O	0	0	0
			958	604	202	151			
53	DU	117	Total	C	N	O	0	0	0
			958	604	202	151			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	BV	101	Total	C	N	O	0	0	0
			779	501	142	135			
54	DV	101	Total	C	N	O	0	0	0
			779	501	142	135			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BW	113	Total	C	N	O	0	0	0
			896	563	176	155			
55	DW	113	Total	C	N	O	0	0	0
			896	563	176	155			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
56	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	107	Total	C	N	O	S	0	0	1
			811	520	155	131	5			
57	DY	107	Total	C	N	O	S	0	0	1
			811	520	155	131	5			

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			
58	DZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total	Mg	0	0
			1	1		
60	CY	1	Total	Mg	0	0
			1	1		

-
- The chemical structure of FUA (Fusaric acid) is a complex polycyclic molecule. It features a central core with several fused and fused rings. Key features include:
- Functional Groups:**
 - A carboxylic acid group (O4, O5) attached to C29.
 - A hydroxyl group (O6) attached to C3.
 - A hydroxyl group (O1) attached to C11.
 - A hydroxyl group (O2) attached to C16.
 - A hydroxyl group (O3) attached to C31.
 - Stereocenters:**
 - C1, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C79

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AY	1	Total C O 37 31 6	0	0
61	CY	1	Total C O 37 31 6	0	0

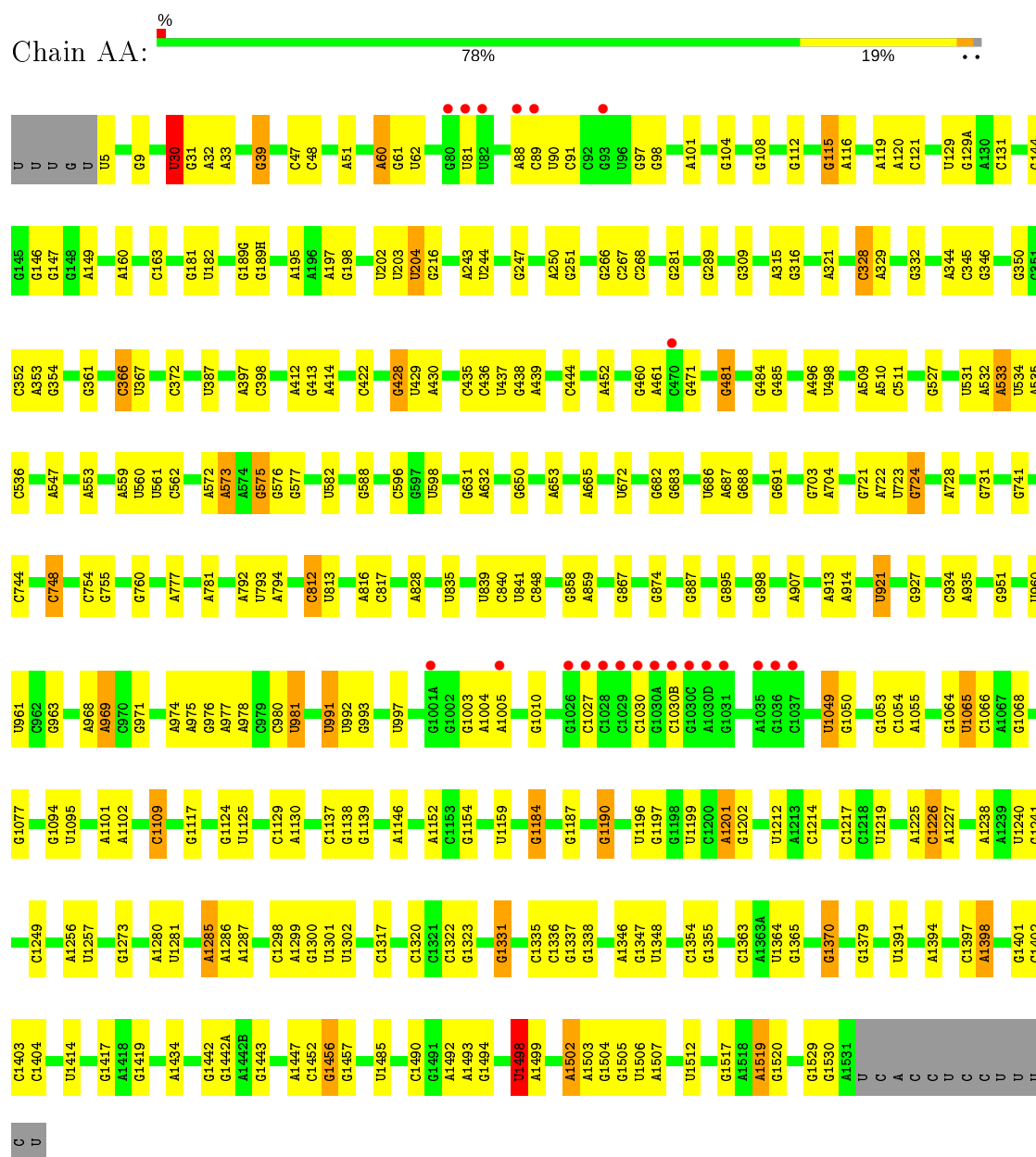
-
- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including the amino group at the 2-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected by a pyrophosphate linkage, with the second phosphate group having a negative charge. The structure is labeled with various atoms and bonds, including the 5' and 3' positions of the ribose sugar and the 1' and 2' positions of the guanine base.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	AY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
62	CY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

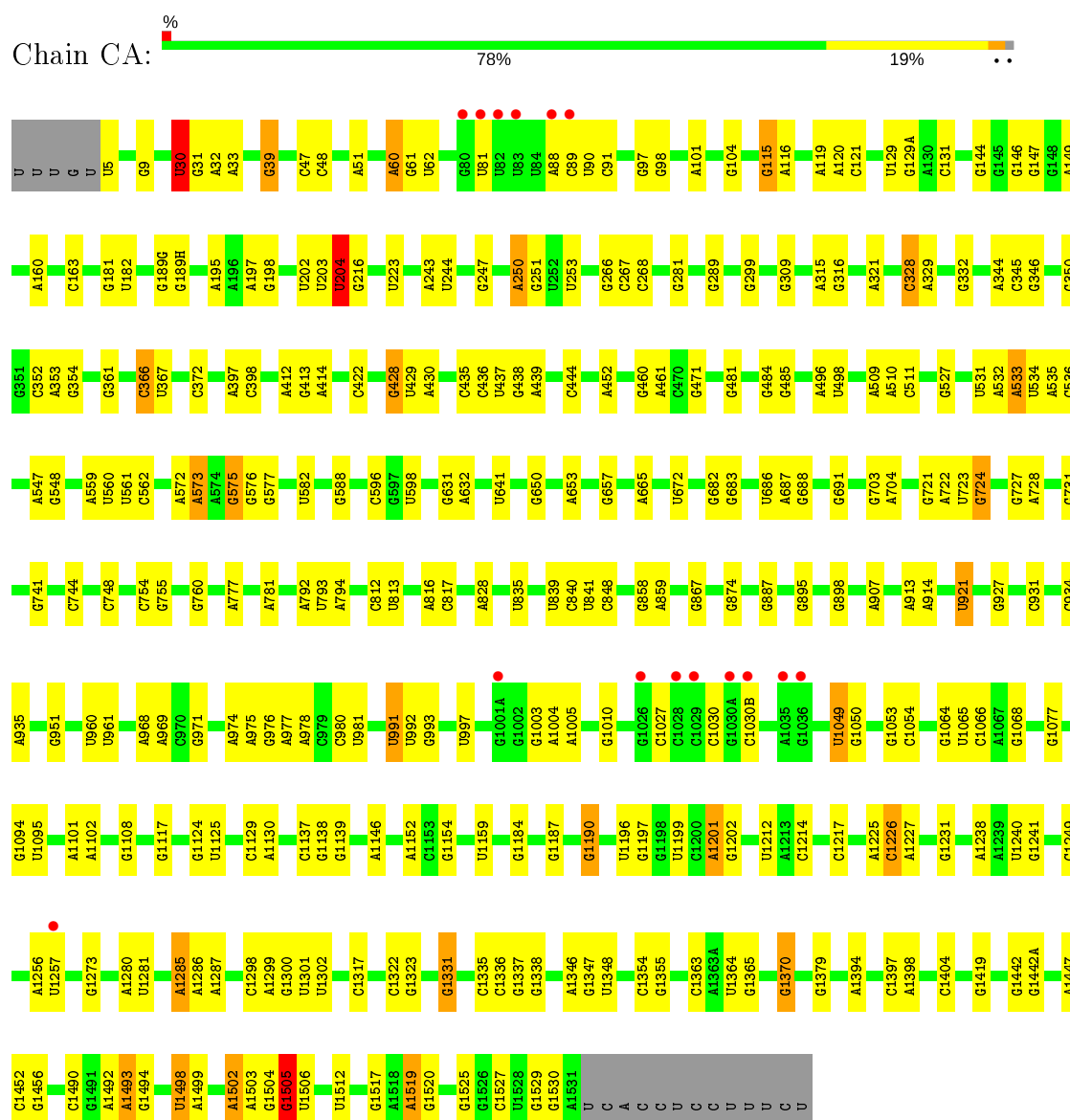
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

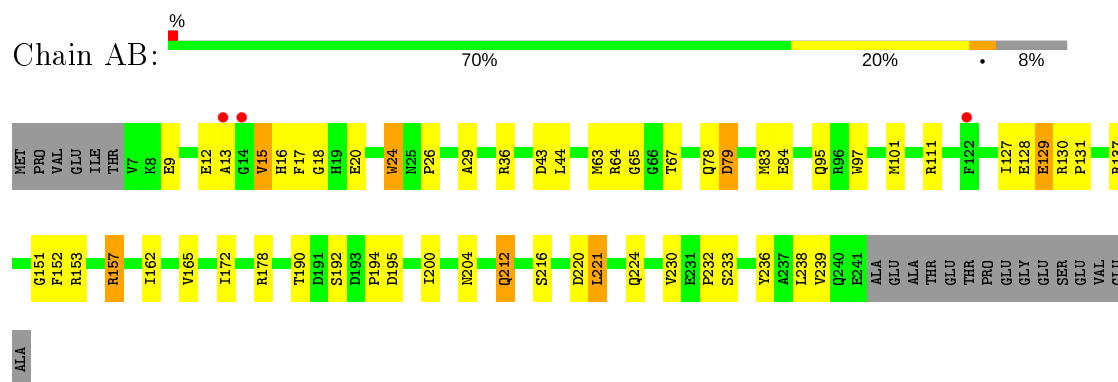
- Molecule 1: 16S ribosomal RNA



- Molecule 1: 16S ribosomal RNA

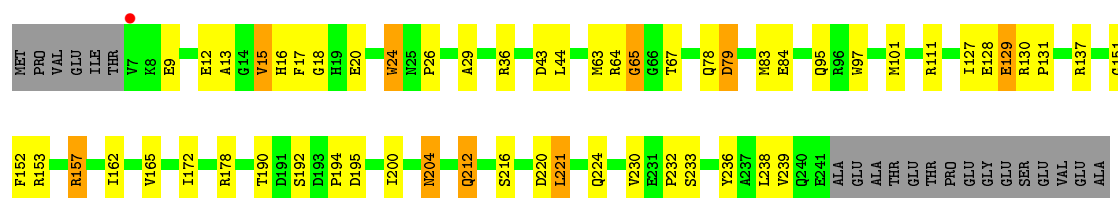


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

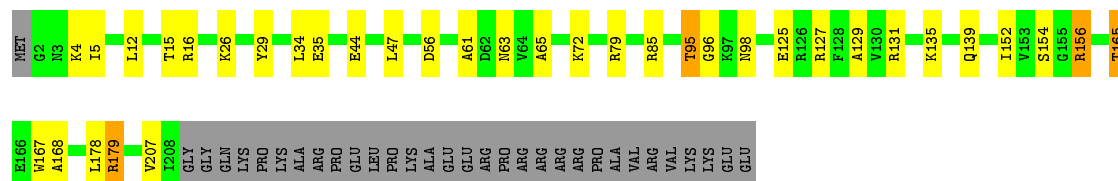


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

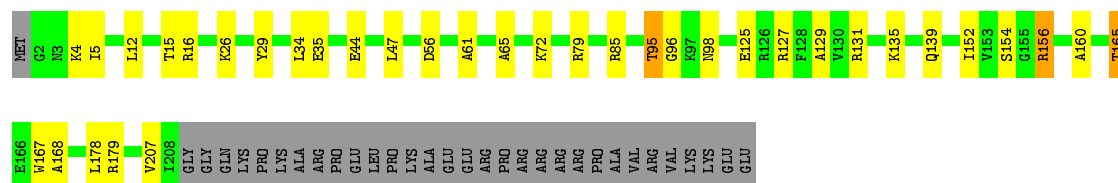




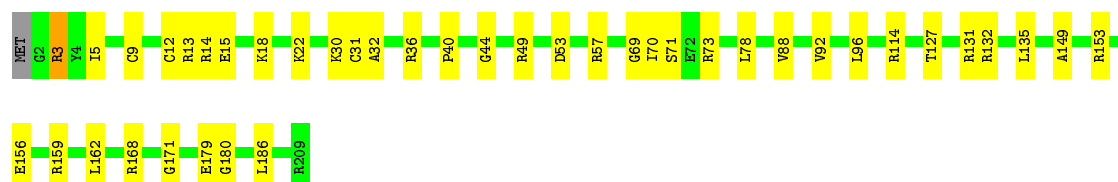
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



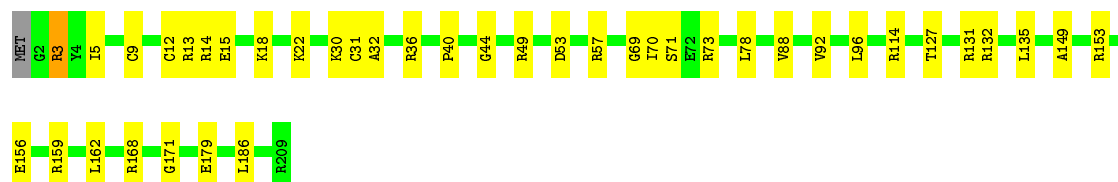
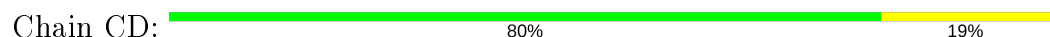
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



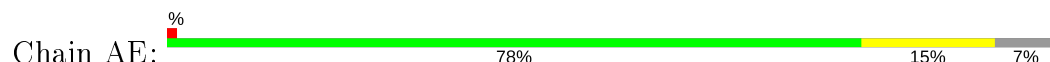
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

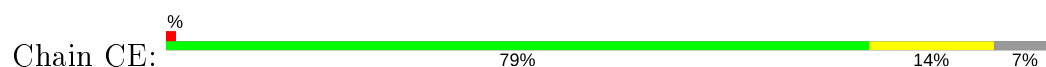


• Molecule 5: 30S RIBOSOMAL PROTEIN S5





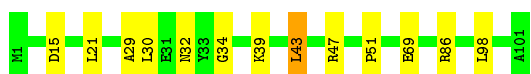
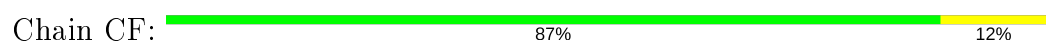
- Molecule 5: 30S RIBOSOMAL PROTEIN S5



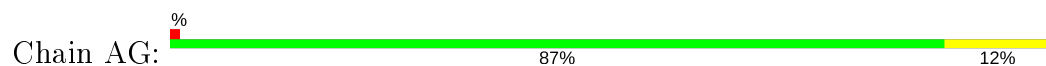
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



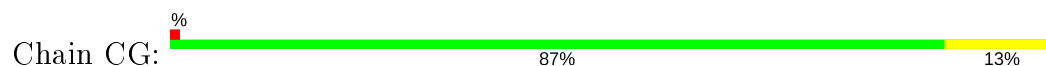
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



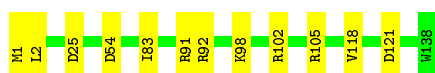
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



- Molecule 7: 30S RIBOSOMAL PROTEIN S7



- Molecule 8: 30S RIBOSOMAL PROTEIN S8

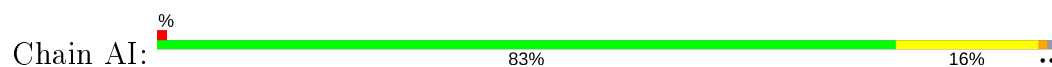


- Molecule 8: 30S RIBOSOMAL PROTEIN S8

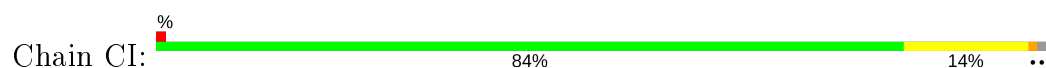




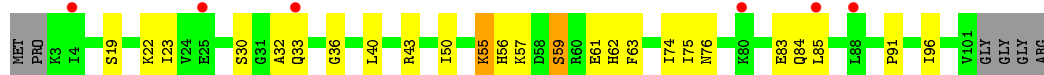
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



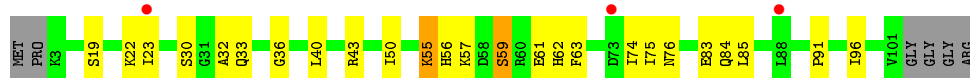
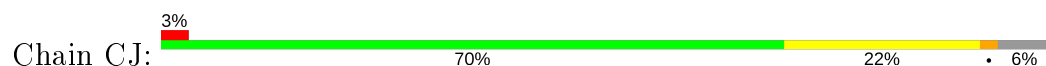
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



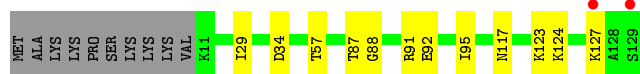
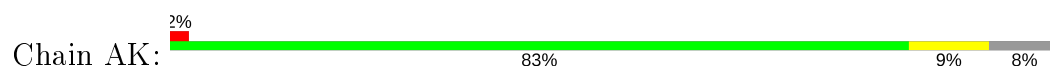
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



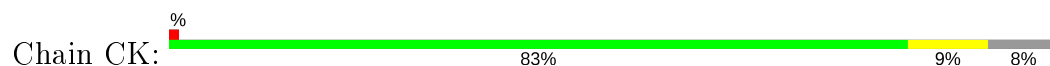
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

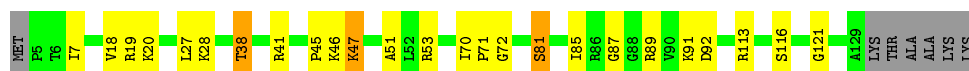


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

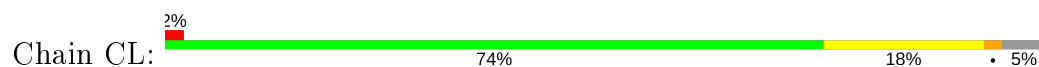


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

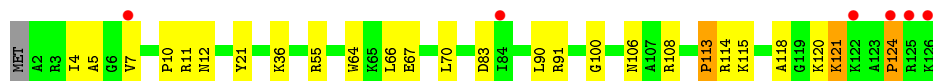
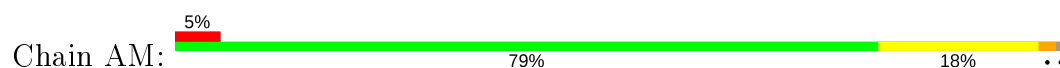




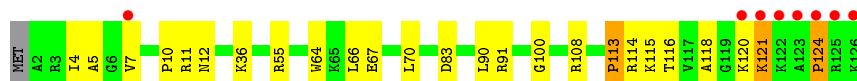
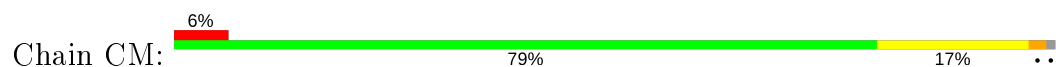
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



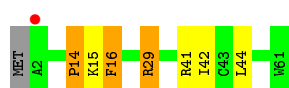
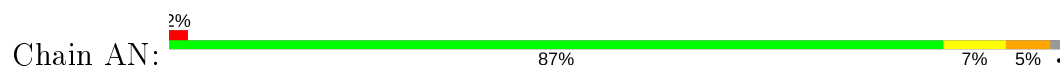
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



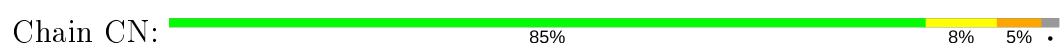
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



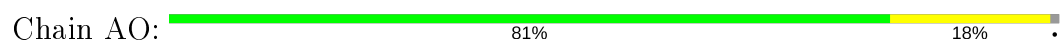
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



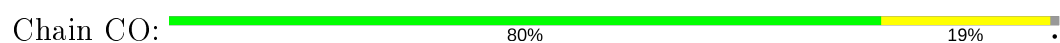
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 15: 30S RIBOSOMAL PROTEIN S15





- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 83% 11% 5%



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP: 83% 11% 5%



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 84% 11% 5%



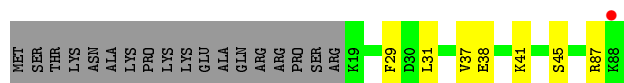
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ: 85% 10% 5%



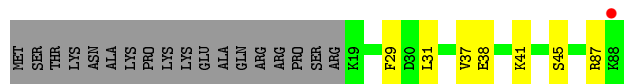
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 72% 8% 20%



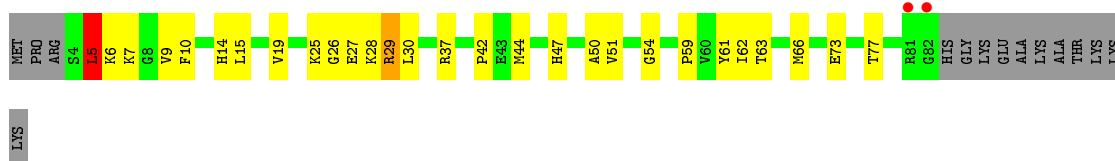
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR: 72% 8% 20%

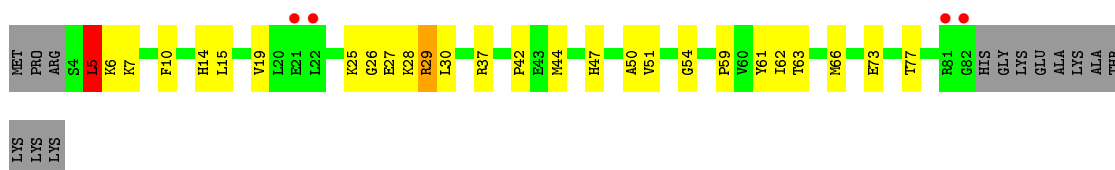


- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS: 55% 28% 15%



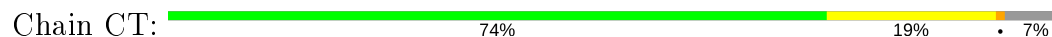
- Molecule 19: 30S RIBOSOMAL PROTEIN S19



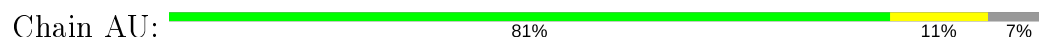
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



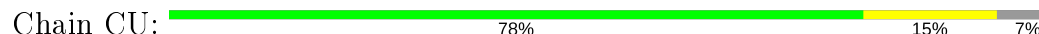
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



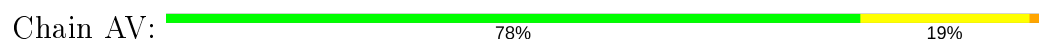
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

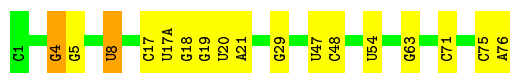


- Molecule 21: 30S RIBOSOMAL PROTEIN THX

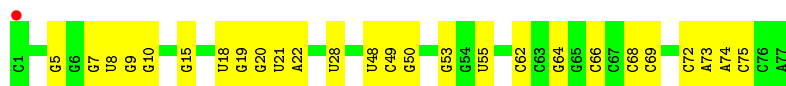


- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)

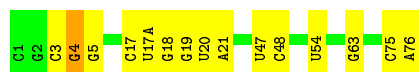
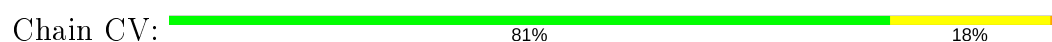




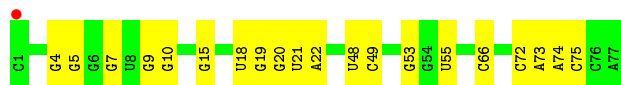
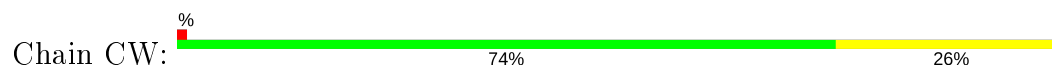
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



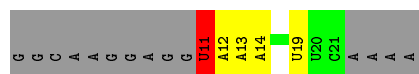
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



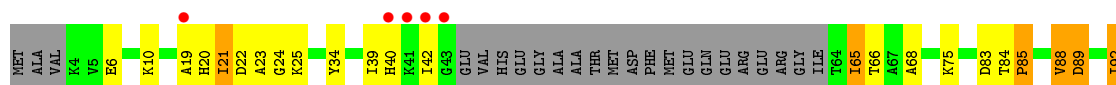
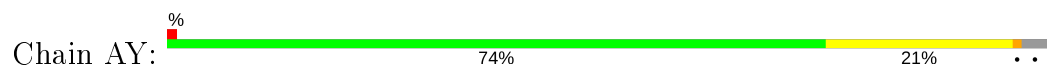
- Molecule 23: MRNA

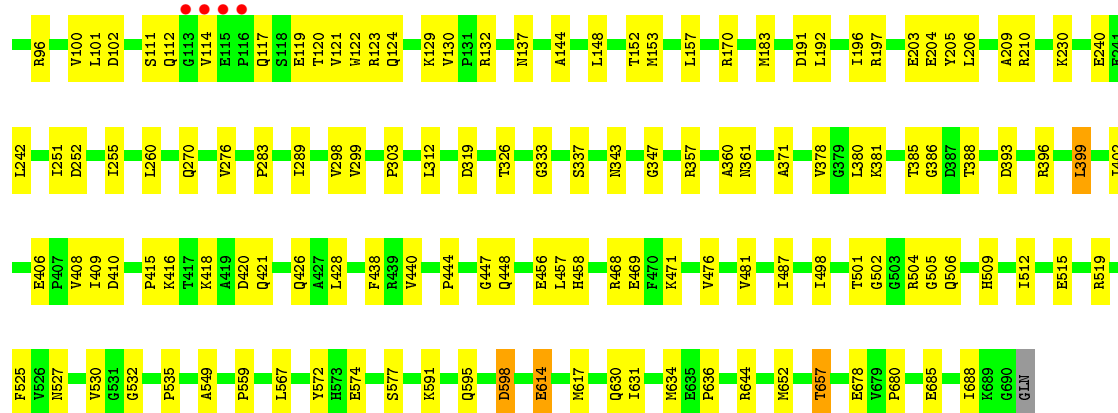


- Molecule 23: MRNA

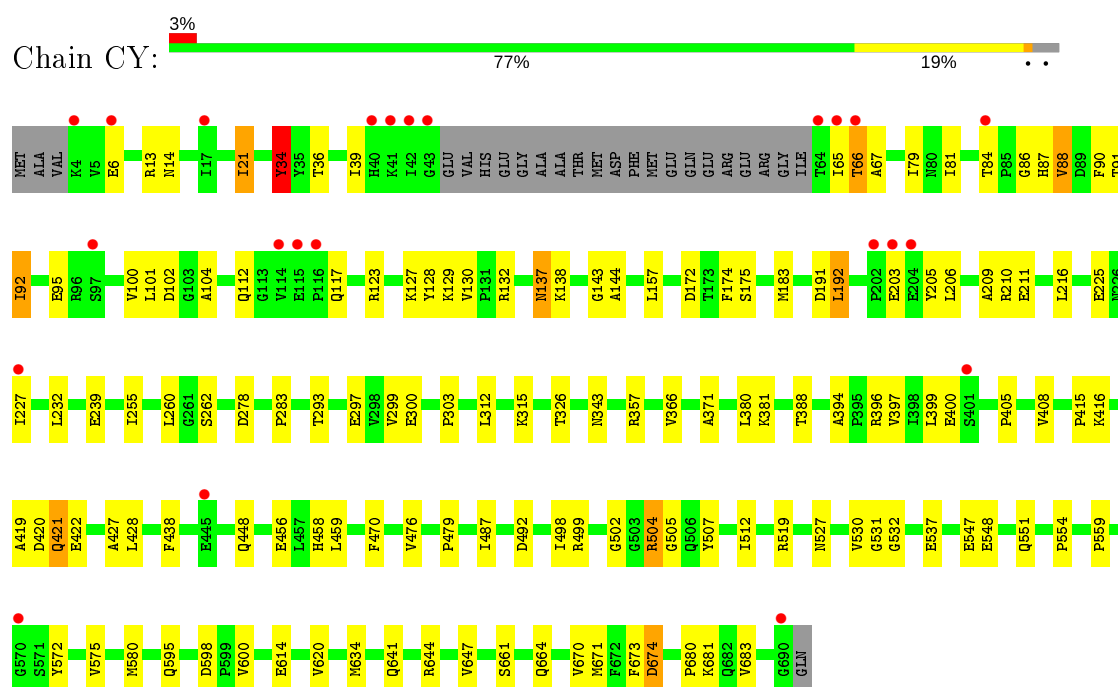


- Molecule 24: ELONGATION FACTOR G

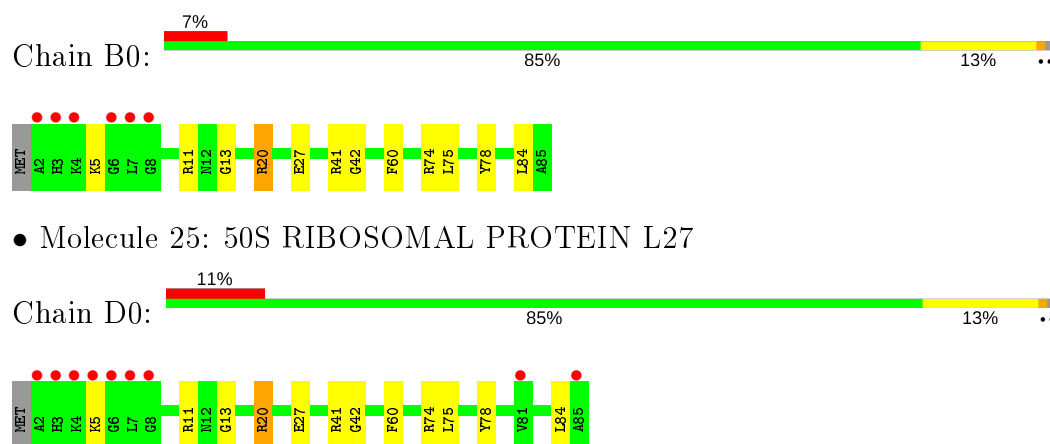




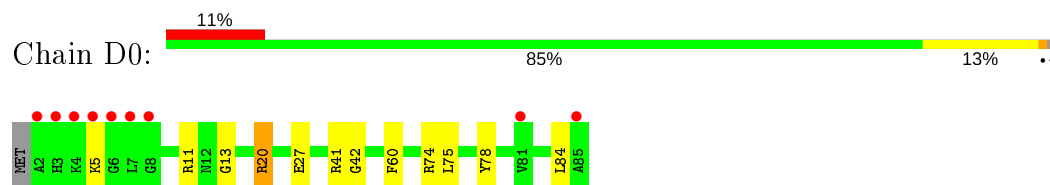
• Molecule 24: ELONGATION FACTOR G



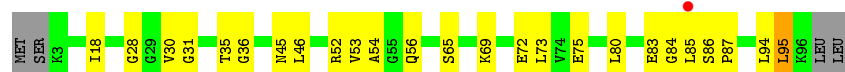
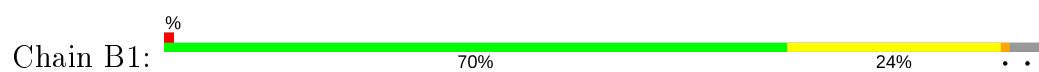
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



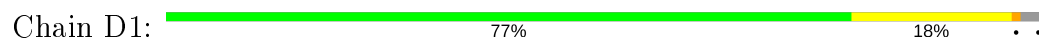
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



• Molecule 26: 50S RIBOSOMAL PROTEIN L28



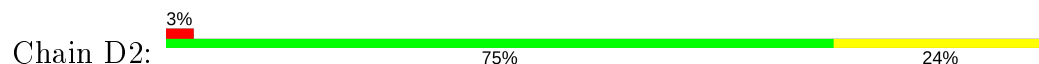
- Molecule 26: 50S RIBOSOMAL PROTEIN L28



- Molecule 27: 50S RIBOSOMAL PROTEIN L29



- Molecule 27: 50S RIBOSOMAL PROTEIN L29



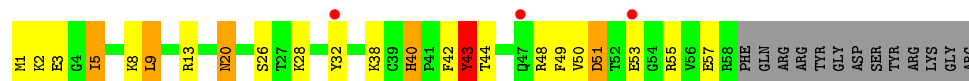
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



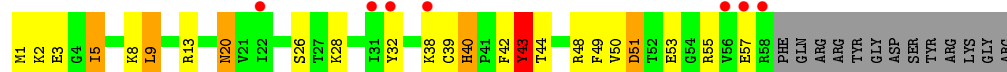
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



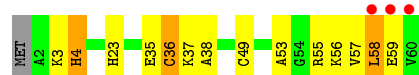
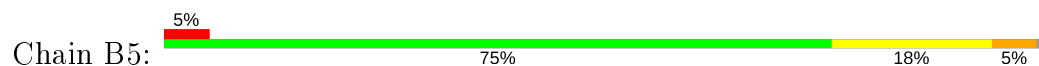
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



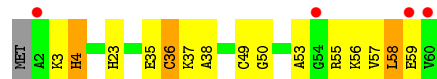
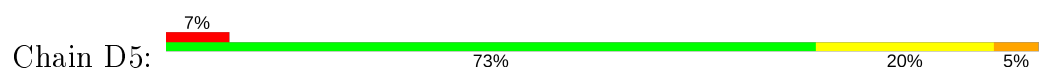
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



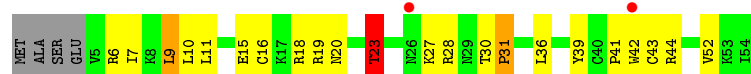
- Molecule 30: 50S RIBOSOMAL PROTEIN L32



- Molecule 30: 50S RIBOSOMAL PROTEIN L32



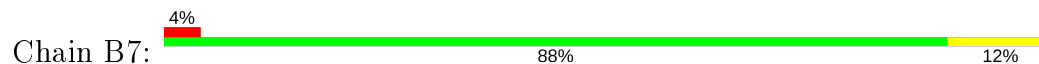
- Molecule 31: 50S RIBOSOMAL PROTEIN L33



- Molecule 31: 50S RIBOSOMAL PROTEIN L33



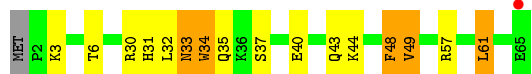
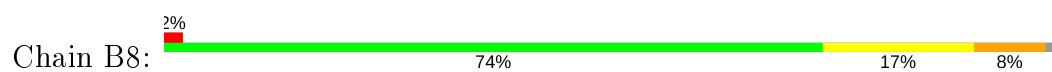
- Molecule 32: 50S RIBOSOMAL PROTEIN L34



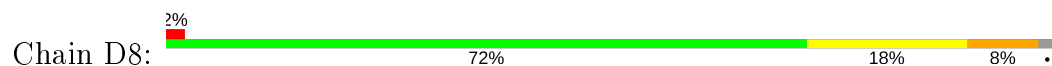
- Molecule 32: 50S RIBOSOMAL PROTEIN L34



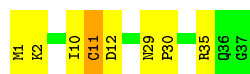
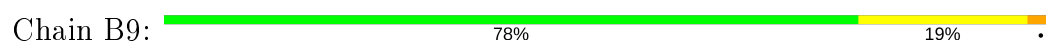
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



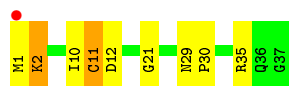
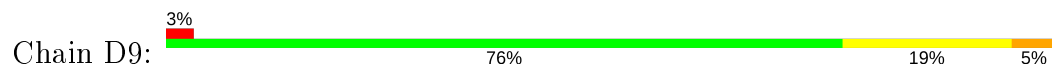
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



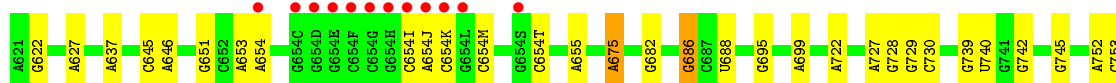
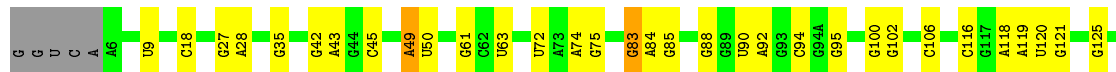
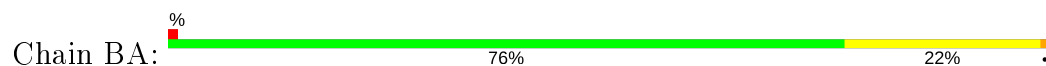
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

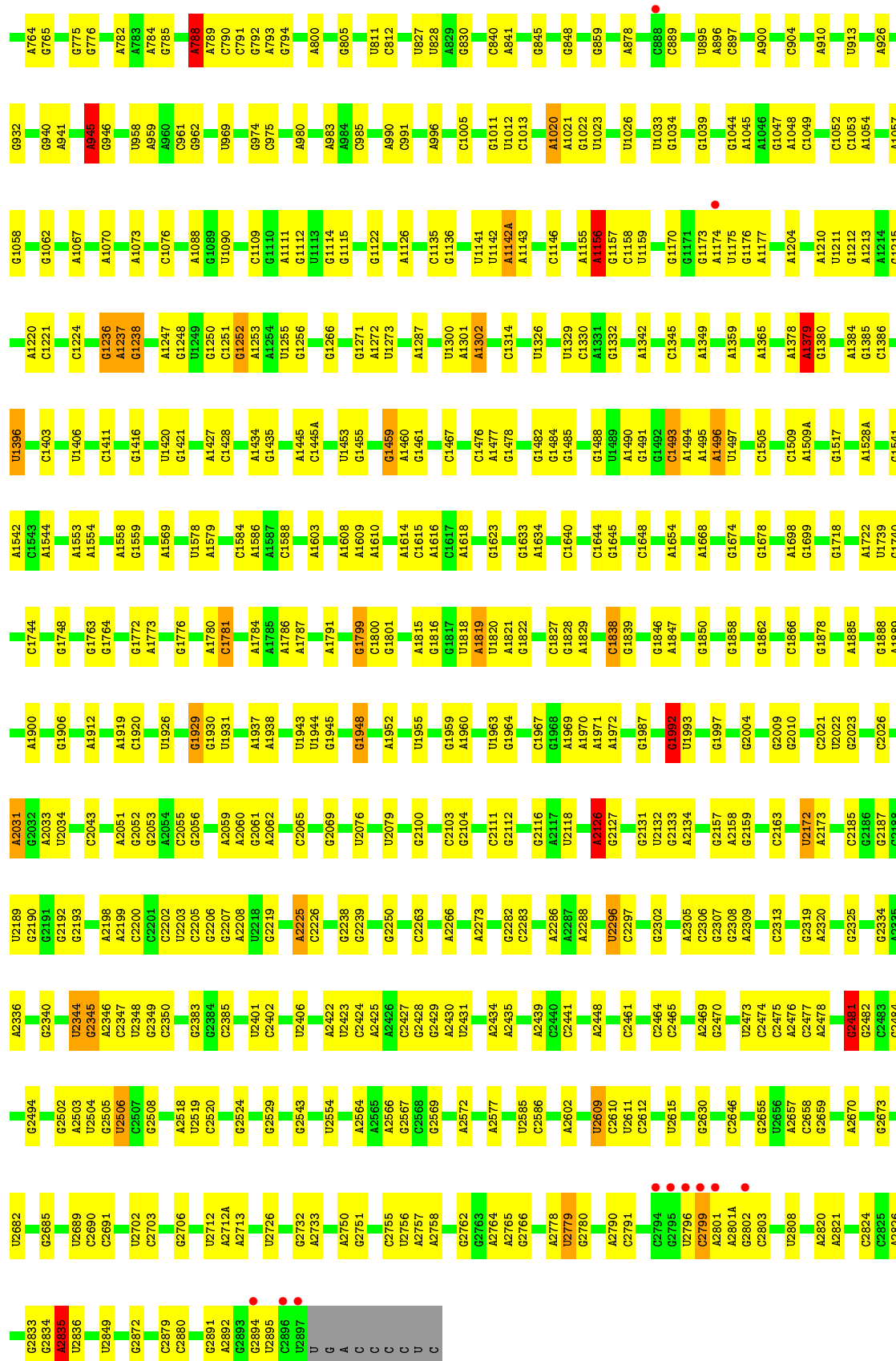


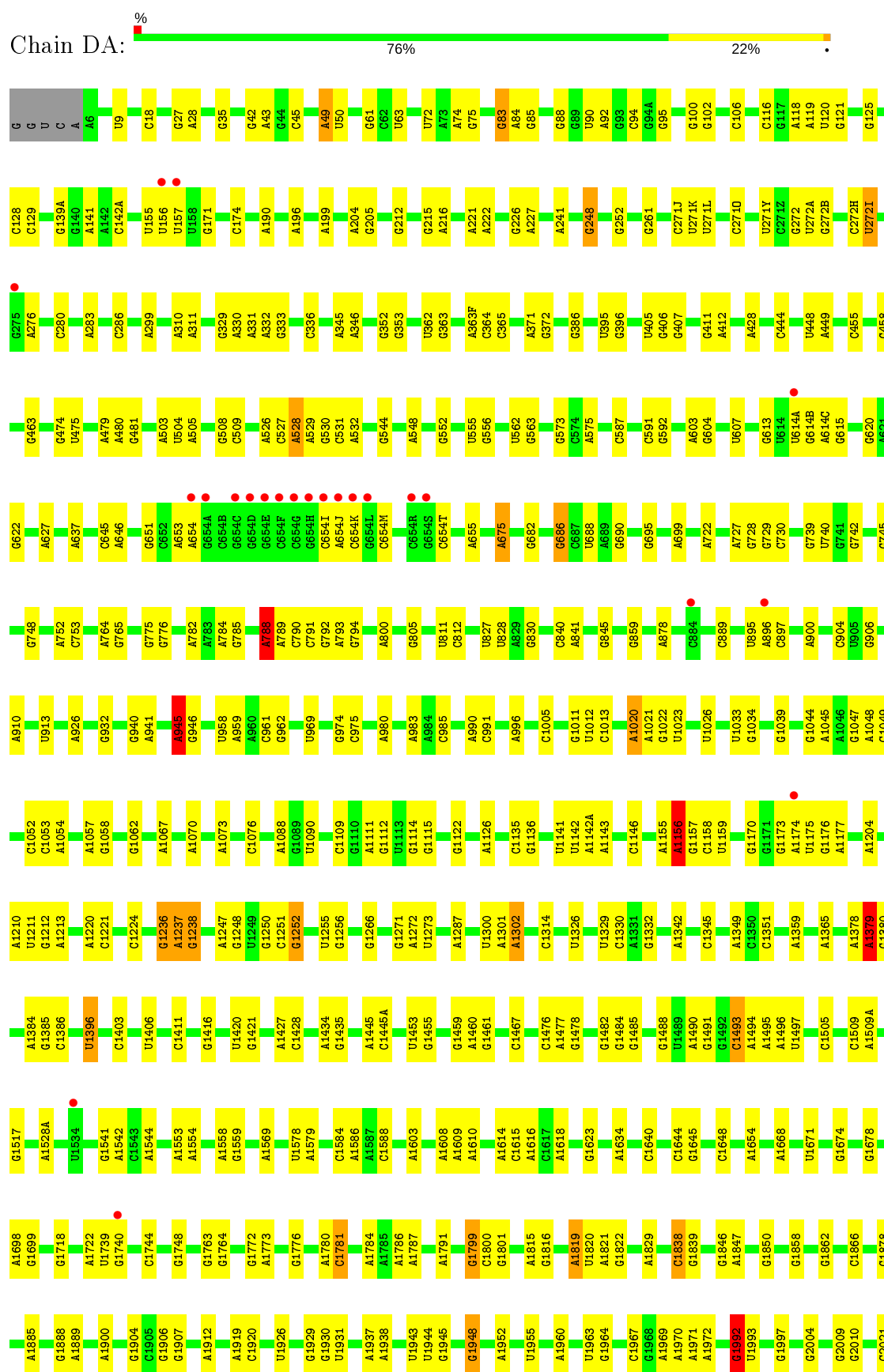
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

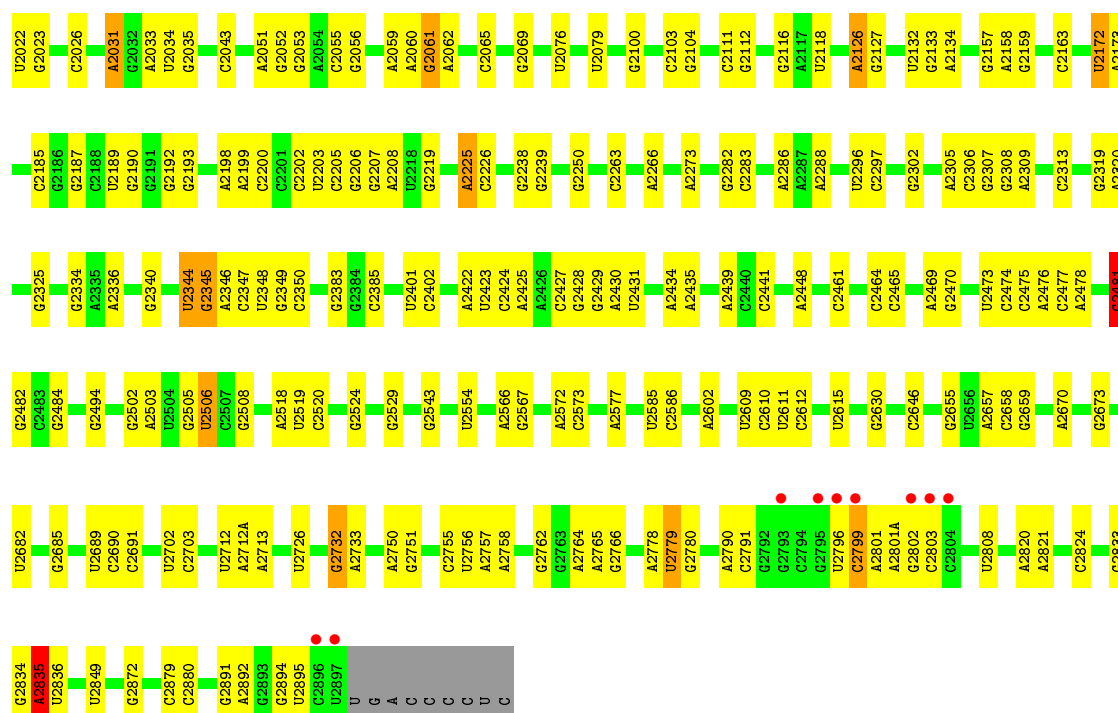


- Molecule 35: 23S RIBOSOMAL RNA









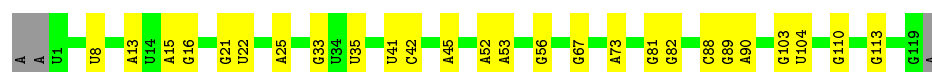
- Molecule 36: 5S RIBOSOMAL RNA

Chain BB: 76% 20%



- Molecule 36: 5S RIBOSOMAL RNA

Chain DB: 76% 21%



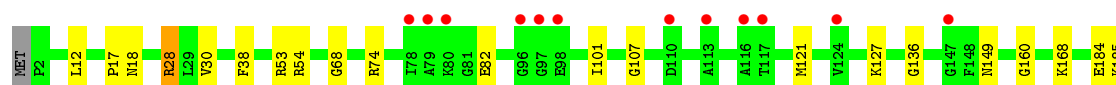
- Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain BC: 2% 90% 10%



- Molecule 37: 50S RIBOSOMAL PROTEIN L1

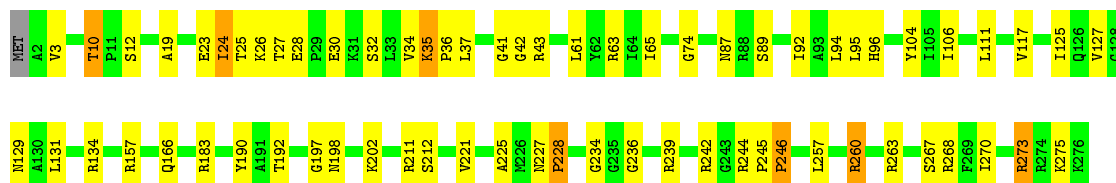
Chain DC: 5% 89% 10%





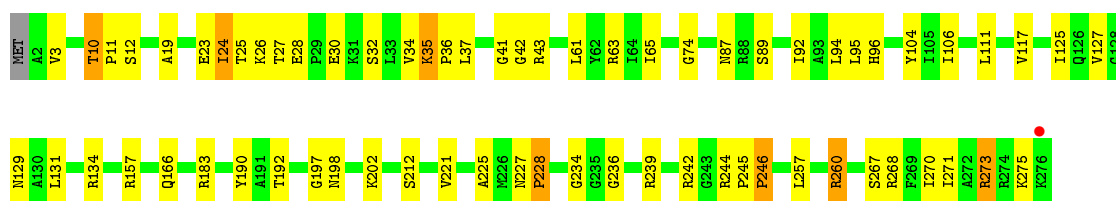
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain BD: 75% 22%



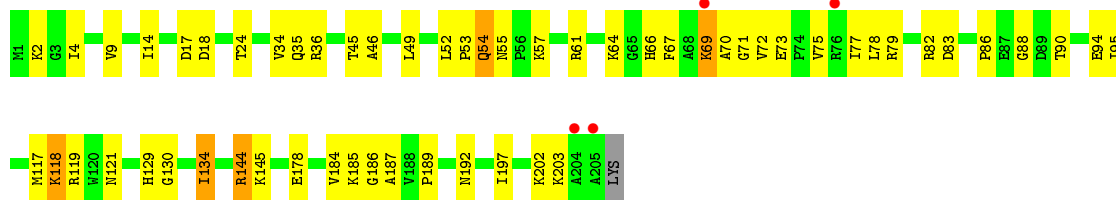
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD: 75% 22%



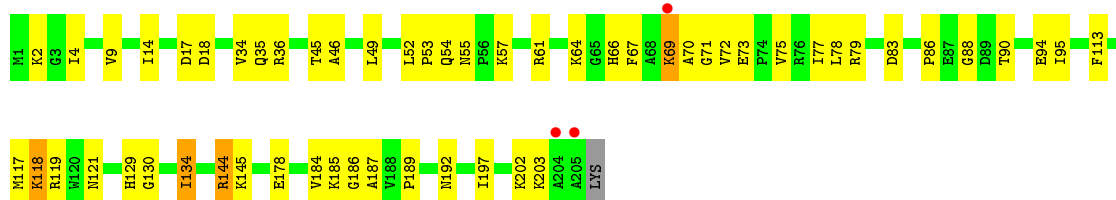
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE: 2% 72% 25%



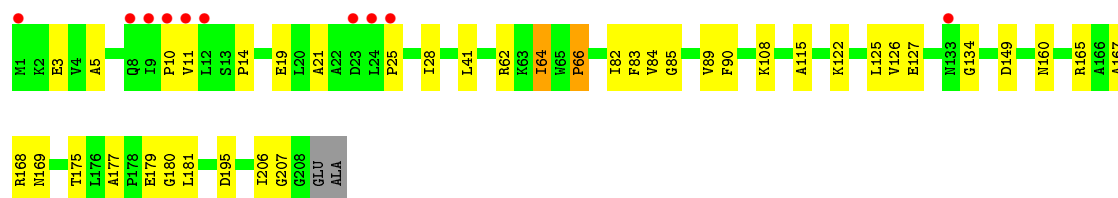
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain DE: 2% 72% 25%

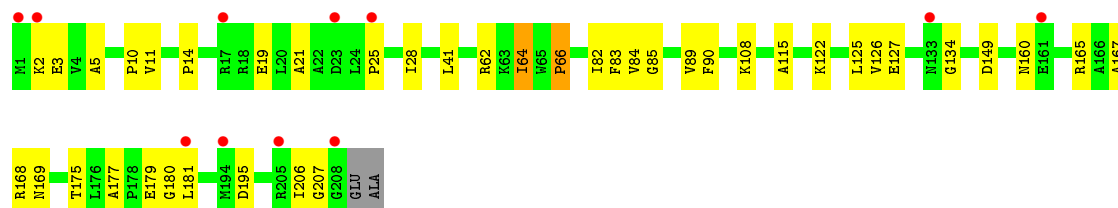
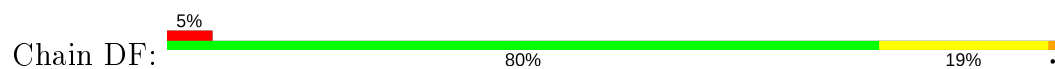


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

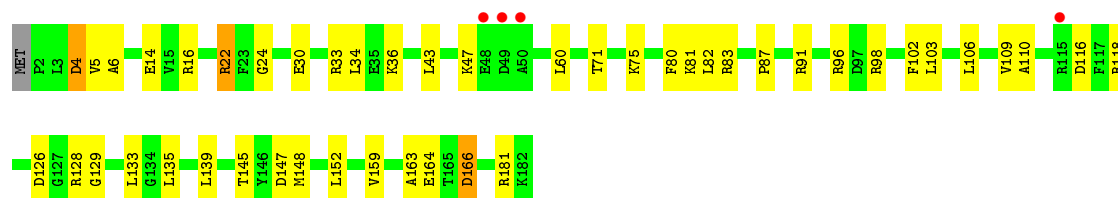
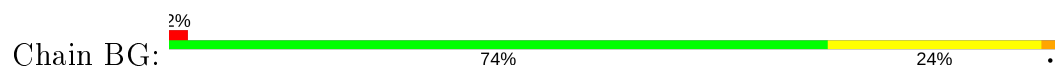
Chain BF: 5% 80% 18%



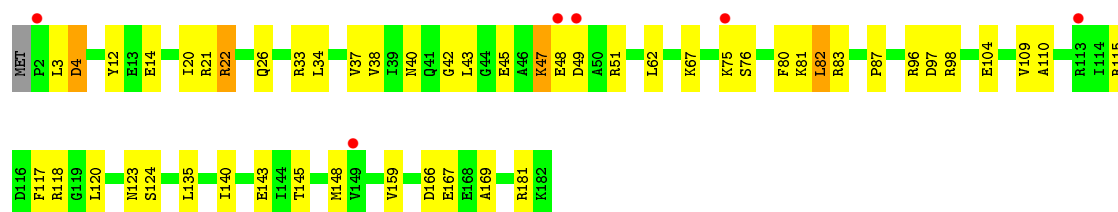
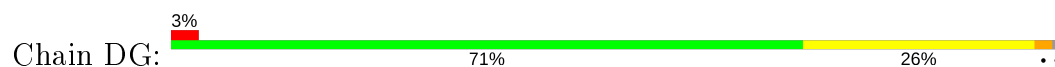
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



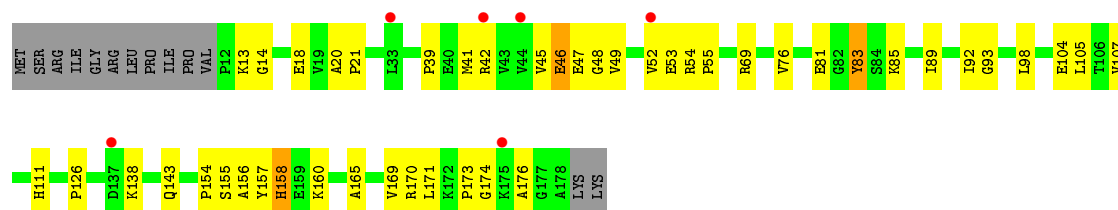
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



• Molecule 41: 50S RIBOSOMAL PROTEIN L5

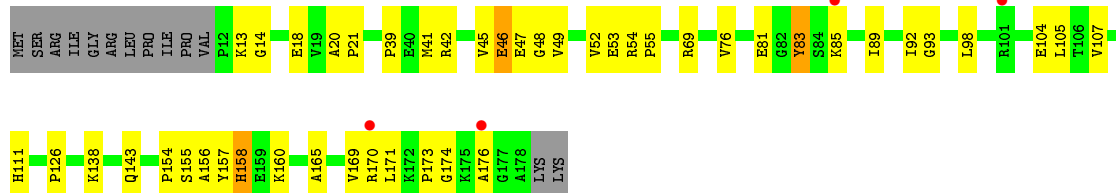


• Molecule 42: 50S RIBOSOMAL PROTEIN L6



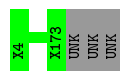
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain DH: 



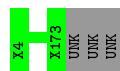
- Molecule 43: 50S RIBOSOMAL PROTEIN L10

Chain BJ: 




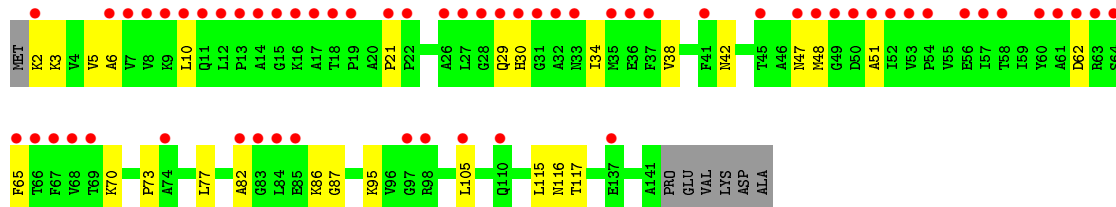
- Molecule 43: 50S RIBOSOMAL PROTEIN L10

Chain DJ: 




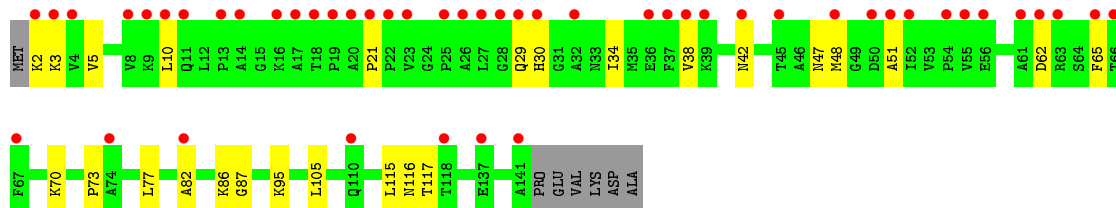
- Molecule 44: 50S RIBOSOMAL PROTEIN L11

Chain BK: 




- Molecule 44: 50S RIBOSOMAL PROTEIN L11

Chain DK: 



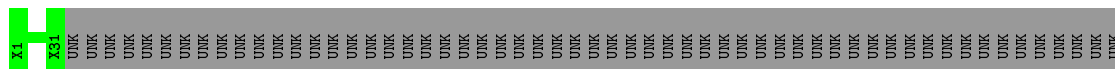
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain BL: 



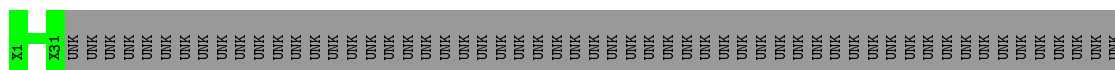
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain BM: 25% 75%



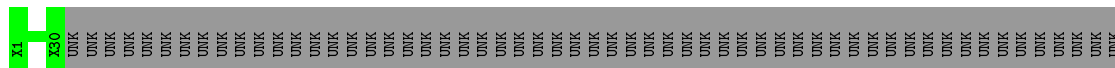
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain BL: 25% 75%



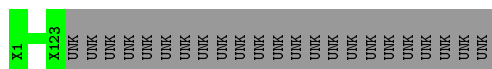
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain Bm: 24% 76%



- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain DL: 82% 18%



- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain DM: 25% 75%



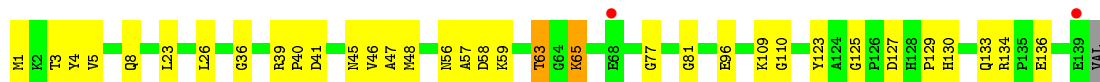
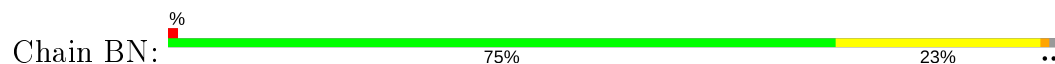
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain DI: 25% 75%

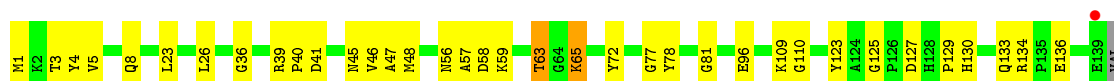
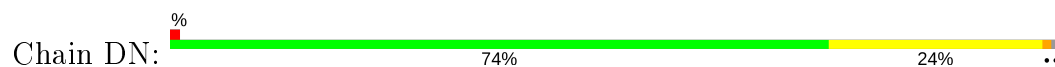
• Molecule 45: 50S RIBOSOMAL PROTEIN L12



- Molecule 46: 50S RIBOSOMAL PROTEIN L13



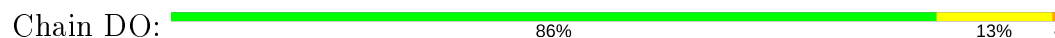
● Molecule 46: 50S RIBOSOMAL PROTEIN L13



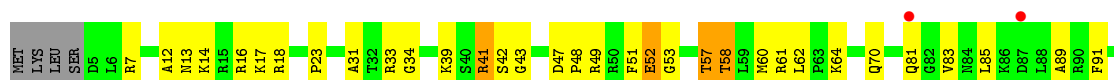
• Molecule 47: 50S RIBOSOMAL PROTEIN L14



- Molecule 47: 50S RIBOSOMAL PROTEIN L14



- Molecule 48: 50S RIBOSOMAL PROTEIN L15

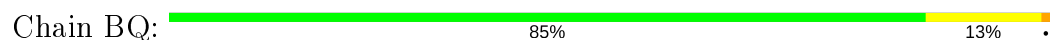




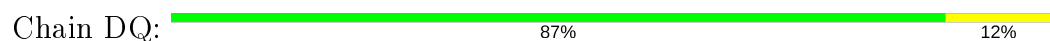
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



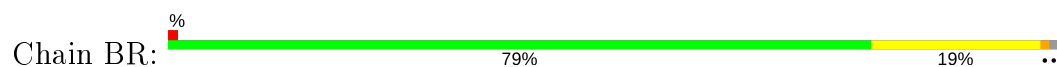
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



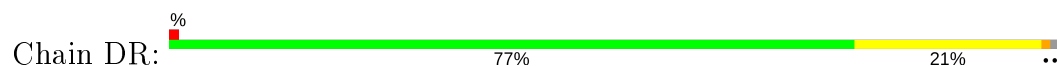
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



• Molecule 50: 50S RIBOSOMAL PROTEIN L17



• Molecule 50: 50S RIBOSOMAL PROTEIN L17

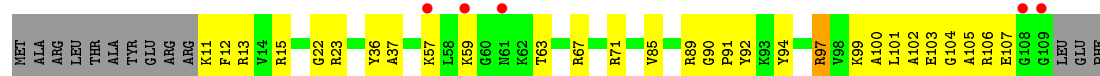


• Molecule 51: 50S RIBOSOMAL PROTEIN L18



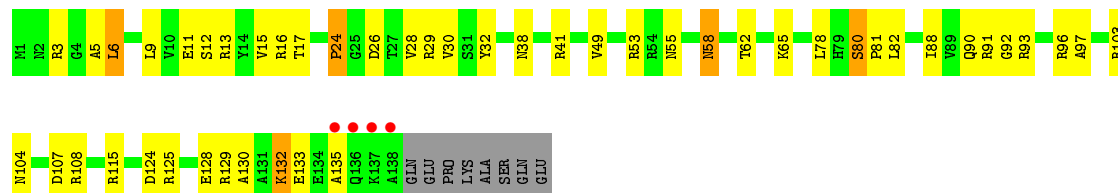
- Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS: 



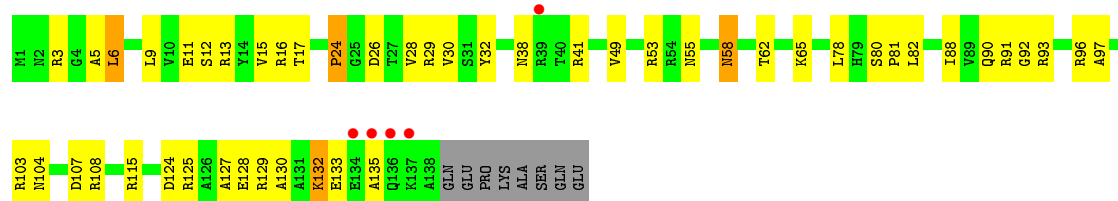
- Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT: 




- Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT: 




- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU: 




- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain DU: 

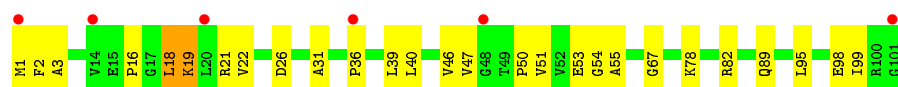
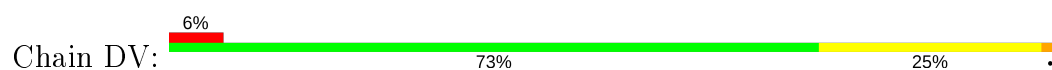


- Molecule 54: 50S RIBOSOMAL PROTEIN L21

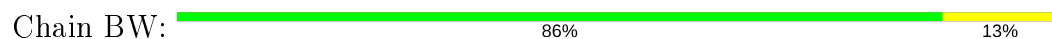
Chain BV: 



- Molecule 54: 50S RIBOSOMAL PROTEIN L21



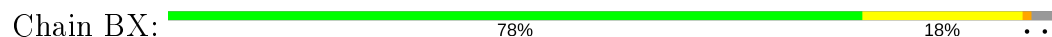
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



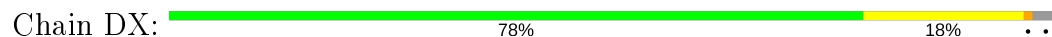
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



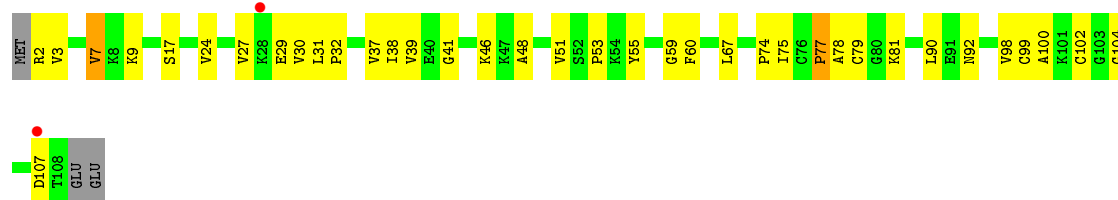
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



- Molecule 56: 50S RIBOSOMAL PROTEIN L23



- Molecule 57: 50S RIBOSOMAL PROTEIN L24



- Molecule 57: 50S RIBOSOMAL PROTEIN L24

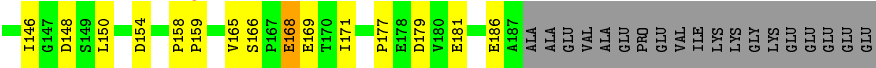




● Molecule 58: 50S RIBOSOMAL PROTEIN L25



● Molecule 58: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	291.84Å 270.36Å 402.36Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 49.57 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-3.60) 95.0 (49.57-3.40)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.260 0.225 , 0.224	Depositor DCC
R_{free} test set	40387 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	311552	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 5MU, ZN, MG, FUA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.61	1/36190 (0.0%)	0.76	26/56486 (0.0%)
1	CA	0.60	2/36190 (0.0%)	0.76	20/56486 (0.0%)
2	AB	0.46	0/1936	0.70	0/2611
2	CB	0.44	0/1936	0.70	0/2611
3	AC	0.52	0/1637	0.69	0/2207
3	CC	0.46	0/1637	0.69	0/2207
4	AD	0.42	0/1733	0.66	0/2318
4	CD	0.41	0/1733	0.66	0/2318
5	AE	0.59	0/1163	0.72	0/1566
5	CE	0.55	0/1163	0.71	0/1566
6	AF	0.44	0/856	0.67	0/1154
6	CF	0.40	0/856	0.66	0/1154
7	AG	0.45	0/1276	0.65	0/1709
7	CG	0.45	0/1276	0.65	0/1709
8	AH	0.51	0/1136	0.74	0/1527
8	CH	0.46	0/1136	0.74	0/1527
9	AI	0.44	0/1027	0.68	0/1373
9	CI	0.41	0/1027	0.67	0/1373
10	AJ	0.47	0/808	0.72	0/1087
10	CJ	0.42	0/808	0.71	0/1087
11	AK	0.50	0/900	0.70	0/1213
11	CK	0.47	0/900	0.70	0/1213
12	AL	0.52	0/987	0.75	0/1322
12	CL	0.48	0/987	0.74	0/1322
13	AM	0.41	0/999	0.69	0/1338
13	CM	0.39	0/999	0.69	0/1338
14	AN	0.49	0/501	0.69	0/664
14	CN	0.47	0/501	0.69	0/664
15	AO	0.45	0/745	0.67	0/992
15	CO	0.43	0/745	0.66	0/992
16	AP	0.45	0/717	0.68	0/965
16	CP	0.43	0/717	0.68	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.51	0/837	0.69	0/1119
17	CQ	0.49	0/837	0.69	0/1119
18	AR	0.47	0/579	0.72	0/768
18	CR	0.45	0/579	0.73	0/768
19	AS	0.46	0/643	0.68	1/867 (0.1%)
19	CS	0.44	0/643	0.67	1/867 (0.1%)
20	AT	0.40	0/765	0.66	0/1007
20	CT	0.39	0/765	0.66	0/1007
21	AU	0.52	0/213	0.65	0/279
21	CU	0.50	0/213	0.65	0/279
22	AV	0.57	0/1810	0.73	0/2821
22	AW	0.41	0/1810	0.72	0/2821
22	CV	0.54	0/1810	0.70	0/2821
22	CW	0.38	0/1810	0.69	0/2821
23	AX	0.82	0/257	0.86	0/398
23	CX	0.79	0/257	0.84	1/398 (0.3%)
24	AY	0.40	0/5313	0.69	0/7195
24	CY	0.42	0/5313	0.69	1/7195 (0.0%)
25	B0	0.43	0/671	0.66	0/892
25	D0	0.42	0/671	0.67	0/892
26	B1	0.48	0/739	0.78	0/983
26	D1	0.45	0/739	0.69	0/983
27	B2	0.36	0/600	0.66	0/793
27	D2	0.37	0/600	0.62	0/793
28	B3	0.43	0/473	0.63	0/636
28	D3	0.43	0/473	0.64	0/636
29	B4	0.68	0/461	0.92	2/623 (0.3%)
29	D4	0.74	0/461	0.93	2/623 (0.3%)
30	B5	0.43	0/473	0.75	0/639
30	D5	0.44	0/473	0.74	0/639
31	B6	0.64	0/440	0.96	1/586 (0.2%)
31	D6	0.64	0/440	0.96	1/586 (0.2%)
32	B7	0.45	0/427	0.71	0/563
32	D7	0.45	0/427	0.71	0/563
33	B8	0.54	0/516	0.83	0/681
33	D8	0.54	0/516	0.83	0/681
34	B9	0.47	0/310	0.69	0/407
34	D9	0.46	0/310	0.70	0/407
35	BA	0.56	3/69972 (0.0%)	0.75	35/109237 (0.0%)
35	DA	0.55	4/69972 (0.0%)	0.75	36/109237 (0.0%)
36	BB	0.44	0/2853	0.72	1/4451 (0.0%)
36	DB	0.44	0/2853	0.72	0/4451
37	BC	0.35	0/1774	0.61	0/2391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.34	0/1774	0.61	0/2391
38	BD	0.54	0/2195	0.83	0/2955
38	DD	0.53	0/2195	0.82	0/2955
39	BE	0.48	0/1597	0.74	0/2155
39	DE	0.46	0/1597	0.74	0/2155
40	BF	0.39	0/1659	0.66	0/2246
40	DF	0.38	0/1659	0.66	0/2246
41	BG	0.42	0/1498	0.78	1/2013 (0.0%)
41	DG	0.43	0/1498	0.74	0/2013
42	BH	0.36	0/1293	0.71	0/1746
42	DH	0.35	0/1293	0.69	0/1746
44	BK	0.35	0/1045	0.60	0/1418
44	DK	0.36	0/1045	0.60	0/1418
46	BN	0.40	0/1132	0.73	1/1527 (0.1%)
46	DN	0.39	0/1132	0.73	1/1527 (0.1%)
47	BO	0.49	0/943	0.72	0/1269
47	DO	0.47	0/943	0.72	0/1269
48	BP	0.44	0/1131	0.93	4/1504 (0.3%)
48	DP	0.44	0/1131	0.91	4/1504 (0.3%)
49	BQ	0.49	0/1143	0.69	0/1527
49	DQ	0.48	0/1143	0.70	0/1527
50	BR	0.39	0/974	0.68	0/1302
50	DR	0.38	0/974	0.68	1/1302 (0.1%)
51	BS	0.41	0/779	0.69	0/1038
51	DS	0.40	0/779	0.70	0/1038
52	BT	0.47	0/1156	0.79	2/1544 (0.1%)
52	DT	0.49	0/1156	0.79	1/1544 (0.1%)
53	BU	0.43	0/975	0.68	0/1297
53	DU	0.44	0/975	0.69	0/1297
54	BV	0.39	0/790	0.70	0/1057
54	DV	0.39	0/790	0.70	0/1057
55	BW	0.37	0/907	0.65	0/1216
55	DW	0.39	0/907	0.65	0/1216
56	BX	0.42	0/740	0.66	0/995
56	DX	0.42	0/740	0.66	0/995
57	BY	0.41	0/824	0.67	0/1100
57	DY	0.42	0/824	0.68	0/1100
58	BZ	0.48	0/1500	0.74	0/2037
58	DZ	0.46	0/1500	0.73	0/2037
All	All	0.53	10/333656 (0.0%)	0.74	143/497270 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	48
1	CA	0	43
22	AV	0	3
22	CV	0	1
23	AX	0	2
23	CX	0	1
35	BA	2	69
35	DA	2	58
36	BB	0	1
36	DB	0	1
37	BC	0	1
37	DC	0	1
44	BK	0	1
44	DK	0	1
46	DN	0	1
All	All	4	232

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	2506	U	N1-C2	7.05	1.44	1.38
35	DA	2506	U	N1-C2	6.48	1.44	1.38
35	BA	272(I)	U	C1'-N1	5.69	1.57	1.48
1	AA	1417	G	C6-O6	5.55	1.29	1.24
35	DA	272(I)	U	C1'-N1	5.49	1.56	1.48

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1992	G	C2'-C3'-O3'	10.77	133.19	109.50
35	DA	1992	G	C2'-C3'-O3'	10.61	132.85	109.50
1	CA	575	G	C2'-C3'-O3'	9.68	130.80	109.50
1	AA	575	G	C2'-C3'-O3'	9.65	130.72	109.50
35	BA	945	A	N9-C1'-C2'	9.34	126.14	114.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	1799	G	C3'
35	BA	1992	G	C3'

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Mol	Chain	Res	Type	Atom
35	DA	1799	G	C3'
35	DA	1992	G	C3'

5 of 232 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	112	G	Sidechain
1	AA	30	U	Sidechain
1	AA	39	G	Sidechain
1	AA	5	U	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	139 (60%)	53 (23%)	41 (18%)	0	2
2	CB	233/256 (91%)	140 (60%)	51 (22%)	42 (18%)	0	2
3	AC	205/239 (86%)	133 (65%)	50 (24%)	22 (11%)	0	7
3	CC	205/239 (86%)	132 (64%)	52 (25%)	21 (10%)	0	7
4	AD	206/209 (99%)	134 (65%)	50 (24%)	22 (11%)	0	7
4	CD	206/209 (99%)	134 (65%)	51 (25%)	21 (10%)	0	7
5	AE	149/162 (92%)	119 (80%)	21 (14%)	9 (6%)	1	17
5	CE	149/162 (92%)	117 (78%)	24 (16%)	8 (5%)	2	19
6	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	14
6	CF	99/101 (98%)	74 (75%)	18 (18%)	7 (7%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	153/156 (98%)	109 (71%)	34 (22%)	10 (6%)	1	16
7	CG	153/156 (98%)	110 (72%)	32 (21%)	11 (7%)	1	13
8	AH	136/138 (99%)	103 (76%)	30 (22%)	3 (2%)	6	39
8	CH	136/138 (99%)	105 (77%)	27 (20%)	4 (3%)	4	33
9	AI	121/128 (94%)	81 (67%)	26 (22%)	14 (12%)	0	6
9	CI	121/128 (94%)	82 (68%)	27 (22%)	12 (10%)	0	8
10	AJ	97/105 (92%)	60 (62%)	21 (22%)	16 (16%)	0	3
10	CJ	97/105 (92%)	61 (63%)	20 (21%)	16 (16%)	0	3
11	AK	117/129 (91%)	91 (78%)	20 (17%)	6 (5%)	2	20
11	CK	117/129 (91%)	91 (78%)	20 (17%)	6 (5%)	2	20
12	AL	123/132 (93%)	82 (67%)	23 (19%)	18 (15%)	0	3
12	CL	123/132 (93%)	82 (67%)	22 (18%)	19 (15%)	0	3
13	AM	123/126 (98%)	77 (63%)	25 (20%)	21 (17%)	0	2
13	CM	123/126 (98%)	77 (63%)	26 (21%)	20 (16%)	0	3
14	AN	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	14
14	CN	58/61 (95%)	46 (79%)	7 (12%)	5 (9%)	1	10
15	AO	86/89 (97%)	55 (64%)	23 (27%)	8 (9%)	0	9
15	CO	86/89 (97%)	53 (62%)	24 (28%)	9 (10%)	0	7
16	AP	82/88 (93%)	60 (73%)	15 (18%)	7 (8%)	1	10
16	CP	82/88 (93%)	60 (73%)	15 (18%)	7 (8%)	1	10
17	AQ	98/105 (93%)	78 (80%)	15 (15%)	5 (5%)	2	20
17	CQ	98/105 (93%)	78 (80%)	16 (16%)	4 (4%)	3	26
18	AR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	1	13
18	CR	68/88 (77%)	51 (75%)	12 (18%)	5 (7%)	1	13
19	AS	77/93 (83%)	43 (56%)	14 (18%)	20 (26%)	0	0
19	CS	77/93 (83%)	43 (56%)	15 (20%)	19 (25%)	0	0
20	AT	97/106 (92%)	52 (54%)	30 (31%)	15 (16%)	0	3
20	CT	97/106 (92%)	53 (55%)	29 (30%)	15 (16%)	0	3
21	AU	23/27 (85%)	14 (61%)	6 (26%)	3 (13%)	0	5
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	2
24	AY	663/691 (96%)	435 (66%)	137 (21%)	91 (14%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	CY	663/691 (96%)	449 (68%)	134 (20%)	80 (12%)	0	5
25	B0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	21
25	D0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	21
26	B1	92/98 (94%)	64 (70%)	15 (16%)	13 (14%)	0	4
26	D1	92/98 (94%)	67 (73%)	13 (14%)	12 (13%)	0	5
27	B2	69/72 (96%)	35 (51%)	18 (26%)	16 (23%)	0	0
27	D2	69/72 (96%)	29 (42%)	31 (45%)	9 (13%)	0	5
28	B3	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1	10
28	D3	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1	10
29	B4	56/71 (79%)	27 (48%)	14 (25%)	15 (27%)	0	0
29	D4	56/71 (79%)	28 (50%)	13 (23%)	15 (27%)	0	0
30	B5	57/60 (95%)	37 (65%)	9 (16%)	11 (19%)	0	2
30	D5	57/60 (95%)	38 (67%)	7 (12%)	12 (21%)	0	1
31	B6	48/54 (89%)	21 (44%)	12 (25%)	15 (31%)	0	0
31	D6	48/54 (89%)	22 (46%)	12 (25%)	14 (29%)	0	0
32	B7	47/49 (96%)	35 (74%)	11 (23%)	1 (2%)	7	40
32	D7	47/49 (96%)	35 (74%)	11 (23%)	1 (2%)	7	40
33	B8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	2
33	D8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	2
34	B9	35/37 (95%)	21 (60%)	9 (26%)	5 (14%)	0	4
34	D9	35/37 (95%)	21 (60%)	8 (23%)	6 (17%)	0	2
37	BC	226/229 (99%)	163 (72%)	51 (23%)	12 (5%)	2	19
37	DC	226/229 (99%)	163 (72%)	50 (22%)	13 (6%)	1	18
38	BD	273/276 (99%)	189 (69%)	50 (18%)	34 (12%)	0	5
38	DD	273/276 (99%)	188 (69%)	50 (18%)	35 (13%)	0	5
39	BE	203/206 (98%)	122 (60%)	45 (22%)	36 (18%)	0	2
39	DE	203/206 (98%)	124 (61%)	44 (22%)	35 (17%)	0	2
40	BF	206/210 (98%)	132 (64%)	44 (21%)	30 (15%)	0	3
40	DF	206/210 (98%)	133 (65%)	42 (20%)	31 (15%)	0	3
41	BG	177/182 (97%)	110 (62%)	43 (24%)	24 (14%)	0	4
41	DG	177/182 (97%)	115 (65%)	36 (20%)	26 (15%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BH	165/180 (92%)	86 (52%)	40 (24%)	39 (24%)	0	0
42	DH	165/180 (92%)	86 (52%)	40 (24%)	39 (24%)	0	0
44	BK	138/147 (94%)	92 (67%)	35 (25%)	11 (8%)	1	11
44	DK	138/147 (94%)	92 (67%)	35 (25%)	11 (8%)	1	11
46	BN	137/140 (98%)	88 (64%)	28 (20%)	21 (15%)	0	3
46	DN	137/140 (98%)	88 (64%)	28 (20%)	21 (15%)	0	3
47	BO	120/122 (98%)	91 (76%)	19 (16%)	10 (8%)	1	10
47	DO	120/122 (98%)	93 (78%)	17 (14%)	10 (8%)	1	10
48	BP	144/150 (96%)	72 (50%)	45 (31%)	27 (19%)	0	2
48	DP	144/150 (96%)	72 (50%)	44 (31%)	28 (19%)	0	2
49	BQ	139/141 (99%)	106 (76%)	26 (19%)	7 (5%)	2	21
49	DQ	139/141 (99%)	106 (76%)	26 (19%)	7 (5%)	2	21
50	BR	115/118 (98%)	81 (70%)	20 (17%)	14 (12%)	0	5
50	DR	115/118 (98%)	81 (70%)	20 (17%)	14 (12%)	0	5
51	BS	97/112 (87%)	41 (42%)	35 (36%)	21 (22%)	0	1
51	DS	97/112 (87%)	41 (42%)	35 (36%)	21 (22%)	0	1
52	BT	136/146 (93%)	76 (56%)	32 (24%)	28 (21%)	0	1
52	DT	136/146 (93%)	75 (55%)	32 (24%)	29 (21%)	0	1
53	BU	115/118 (98%)	66 (57%)	37 (32%)	12 (10%)	0	7
53	DU	115/118 (98%)	67 (58%)	35 (30%)	13 (11%)	0	6
54	BV	99/101 (98%)	69 (70%)	12 (12%)	18 (18%)	0	2
54	DV	99/101 (98%)	69 (70%)	12 (12%)	18 (18%)	0	2
55	BW	111/113 (98%)	80 (72%)	21 (19%)	10 (9%)	1	9
55	DW	111/113 (98%)	81 (73%)	21 (19%)	9 (8%)	1	11
56	BX	91/96 (95%)	56 (62%)	26 (29%)	9 (10%)	0	8
56	DX	91/96 (95%)	57 (63%)	25 (28%)	9 (10%)	0	8
57	BY	105/110 (96%)	42 (40%)	36 (34%)	27 (26%)	0	0
57	DY	105/110 (96%)	43 (41%)	36 (34%)	26 (25%)	0	0
58	BZ	183/206 (89%)	108 (59%)	42 (23%)	33 (18%)	0	2
58	DZ	183/206 (89%)	114 (62%)	37 (20%)	32 (18%)	0	2
All	All	13200/13966 (94%)	8607 (65%)	2874 (22%)	1719 (13%)	0	5

5 of 1719 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	GLU
2	AB	13	ALA
2	AB	15	VAL
2	AB	20	GLU
2	AB	95	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	179 (89%)	23 (11%)	5	29
2	CB	202/220 (92%)	179 (89%)	23 (11%)	5	29
3	AC	160/188 (85%)	142 (89%)	18 (11%)	6	30
3	CC	160/188 (85%)	142 (89%)	18 (11%)	6	30
4	AD	180/181 (99%)	160 (89%)	20 (11%)	6	31
4	CD	180/181 (99%)	160 (89%)	20 (11%)	6	31
5	AE	115/123 (94%)	100 (87%)	15 (13%)	4	24
5	CE	115/123 (94%)	100 (87%)	15 (13%)	4	24
6	AF	90/90 (100%)	83 (92%)	7 (8%)	12	44
6	CF	90/90 (100%)	83 (92%)	7 (8%)	12	44
7	AG	126/127 (99%)	117 (93%)	9 (7%)	14	48
7	CG	126/127 (99%)	117 (93%)	9 (7%)	14	48
8	AH	119/119 (100%)	110 (92%)	9 (8%)	13	45
8	CH	119/119 (100%)	112 (94%)	7 (6%)	19	55
9	AI	98/99 (99%)	90 (92%)	8 (8%)	11	42
9	CI	98/99 (99%)	90 (92%)	8 (8%)	11	42
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	4	25
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	4	25
11	AK	90/99 (91%)	84 (93%)	6 (7%)	16	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	CK	90/99 (91%)	84 (93%)	6 (7%)	16	50
12	AL	104/109 (95%)	94 (90%)	10 (10%)	8	37
12	CL	104/109 (95%)	93 (89%)	11 (11%)	6	32
13	AM	99/101 (98%)	91 (92%)	8 (8%)	11	43
13	CM	99/101 (98%)	91 (92%)	8 (8%)	11	43
14	AN	49/50 (98%)	43 (88%)	6 (12%)	5	26
14	CN	49/50 (98%)	43 (88%)	6 (12%)	5	26
15	AO	79/80 (99%)	71 (90%)	8 (10%)	7	34
15	CO	79/80 (99%)	71 (90%)	8 (10%)	7	34
16	AP	72/74 (97%)	67 (93%)	5 (7%)	15	49
16	CP	72/74 (97%)	67 (93%)	5 (7%)	15	49
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	46
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	46
18	AR	61/77 (79%)	59 (97%)	2 (3%)	38	69
18	CR	61/77 (79%)	59 (97%)	2 (3%)	38	69
19	AS	69/80 (86%)	59 (86%)	10 (14%)	3	20
19	CS	69/80 (86%)	59 (86%)	10 (14%)	3	20
20	AT	76/82 (93%)	69 (91%)	7 (9%)	9	39
20	CT	76/82 (93%)	69 (91%)	7 (9%)	9	39
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
24	AY	563/582 (97%)	489 (87%)	74 (13%)	4	23
24	CY	563/582 (97%)	495 (88%)	68 (12%)	5	26
25	B0	66/67 (98%)	57 (86%)	9 (14%)	3	22
25	D0	66/67 (98%)	57 (86%)	9 (14%)	3	22
26	B1	78/83 (94%)	65 (83%)	13 (17%)	2	14
26	D1	78/83 (94%)	70 (90%)	8 (10%)	7	34
27	B2	66/67 (98%)	59 (89%)	7 (11%)	6	32
27	D2	66/67 (98%)	58 (88%)	8 (12%)	5	26
28	B3	51/52 (98%)	47 (92%)	4 (8%)	12	44
28	D3	51/52 (98%)	47 (92%)	4 (8%)	12	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	B4	51/63 (81%)	38 (74%)	13 (26%)	0	4
29	D4	51/63 (81%)	37 (72%)	14 (28%)	0	3
30	B5	51/52 (98%)	45 (88%)	6 (12%)	5	28
30	D5	51/52 (98%)	45 (88%)	6 (12%)	5	28
31	B6	49/52 (94%)	39 (80%)	10 (20%)	1	8
31	D6	49/52 (94%)	38 (78%)	11 (22%)	1	6
32	B7	41/42 (98%)	36 (88%)	5 (12%)	5	26
32	D7	41/42 (98%)	36 (88%)	5 (12%)	5	26
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	14
33	D8	53/55 (96%)	43 (81%)	10 (19%)	1	9
34	B9	34/34 (100%)	30 (88%)	4 (12%)	5	28
34	D9	34/34 (100%)	29 (85%)	5 (15%)	3	20
37	BC	180/181 (99%)	170 (94%)	10 (6%)	21	56
37	DC	180/181 (99%)	169 (94%)	11 (6%)	18	53
38	BD	217/218 (100%)	177 (82%)	40 (18%)	1	10
38	DD	217/218 (100%)	178 (82%)	39 (18%)	1	11
39	BE	165/166 (99%)	139 (84%)	26 (16%)	2	17
39	DE	165/166 (99%)	140 (85%)	25 (15%)	3	19
40	BF	165/166 (99%)	153 (93%)	12 (7%)	14	46
40	DF	165/166 (99%)	153 (93%)	12 (7%)	14	46
41	BG	155/156 (99%)	131 (84%)	24 (16%)	2	18
41	DG	155/156 (99%)	126 (81%)	29 (19%)	1	10
42	BH	136/148 (92%)	126 (93%)	10 (7%)	13	46
42	DH	136/148 (92%)	126 (93%)	10 (7%)	13	46
44	BK	104/111 (94%)	89 (86%)	15 (14%)	3	20
44	DK	104/111 (94%)	90 (86%)	14 (14%)	4	23
46	BN	117/119 (98%)	103 (88%)	14 (12%)	5	27
46	DN	117/119 (98%)	102 (87%)	15 (13%)	4	24
47	BO	100/100 (100%)	92 (92%)	8 (8%)	12	43
47	DO	100/100 (100%)	92 (92%)	8 (8%)	12	43
48	BP	112/116 (97%)	91 (81%)	21 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	DP	112/116 (97%)	91 (81%)	21 (19%)	1	9
49	BQ	111/111 (100%)	95 (86%)	16 (14%)	3	20
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	4	24
50	BR	100/101 (99%)	89 (89%)	11 (11%)	6	31
50	DR	100/101 (99%)	88 (88%)	12 (12%)	5	27
51	BS	77/88 (88%)	68 (88%)	9 (12%)	5	29
51	DS	77/88 (88%)	68 (88%)	9 (12%)	5	29
52	BT	120/127 (94%)	97 (81%)	23 (19%)	1	9
52	DT	120/127 (94%)	97 (81%)	23 (19%)	1	9
53	BU	92/94 (98%)	83 (90%)	9 (10%)	8	36
53	DU	92/94 (98%)	83 (90%)	9 (10%)	8	36
54	BV	82/82 (100%)	71 (87%)	11 (13%)	4	23
54	DV	82/82 (100%)	71 (87%)	11 (13%)	4	23
55	BW	91/92 (99%)	84 (92%)	7 (8%)	13	45
55	DW	91/92 (99%)	84 (92%)	7 (8%)	13	45
56	BX	74/78 (95%)	64 (86%)	10 (14%)	4	23
56	DX	74/78 (95%)	64 (86%)	10 (14%)	4	23
57	BY	87/91 (96%)	75 (86%)	12 (14%)	3	22
57	DY	87/91 (96%)	75 (86%)	12 (14%)	3	22
58	BZ	162/179 (90%)	134 (83%)	28 (17%)	2	12
58	DZ	162/179 (90%)	144 (89%)	18 (11%)	6	31
All	All	11080/11566 (96%)	9776 (88%)	1304 (12%)	5	28

5 of 1304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	BU	108	GLU
5	CE	75	THR
51	DS	11	LYS
55	BW	98	LYS
2	CB	24	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 348 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	94	ASN
6	CF	27	GLN
50	DR	23	ASN
56	BX	41	ASN
2	CB	204	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	270 (17%)	43 (2%)
1	CA	1503/1522 (98%)	266 (17%)	43 (2%)
22	AV	76/77 (98%)	15 (19%)	0
22	AW	76/77 (98%)	25 (32%)	1 (1%)
22	CV	76/77 (98%)	14 (18%)	0
22	CW	76/77 (98%)	19 (25%)	1 (1%)
23	AX	11/25 (44%)	4 (36%)	1 (9%)
23	CX	11/25 (44%)	4 (36%)	1 (9%)
35	BA	2900/2915 (99%)	597 (20%)	71 (2%)
35	DA	2900/2915 (99%)	594 (20%)	71 (2%)
36	BB	118/122 (96%)	25 (21%)	0
36	DB	118/122 (96%)	25 (21%)	0
All	All	9368/9476 (98%)	1858 (19%)	232 (2%)

5 of 1858 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	33	A
1	AA	39	G

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2611	U
1	CA	428	G
35	DA	2344	U
35	BA	2762	G
1	CA	60	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	5MU	AV	54	22	14,21,23	1.25	2 (14%)	14,30,35	1.08	1 (7%)
22	5MU	CV	54	22	14,21,23	1.19	2 (14%)	14,30,35	1.12	1 (7%)
22	5MU	AW	55	22	14,21,23	1.24	2 (14%)	14,30,35	1.13	1 (7%)
22	5MU	CW	55	22	14,21,23	1.24	2 (14%)	14,30,35	1.12	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	AV	54	22	-	0/5/25/26	0/2/2/2
22	5MU	CV	54	22	-	0/5/25/26	0/2/2/2
22	5MU	AW	55	22	-	0/5/25/26	0/2/2/2
22	5MU	CW	55	22	-	0/5/25/26	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AW	55	5MU	C4-N3	3.47	1.39	1.33
22	CW	55	5MU	C4-N3	3.38	1.38	1.33
22	AV	54	5MU	C4-N3	3.33	1.38	1.33
22	CV	54	5MU	C4-N3	3.25	1.38	1.33
22	AV	54	5MU	C6-N1	2.28	1.38	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AW	55	5MU	C5-C4-N3	-3.69	115.19	123.31
22	CV	54	5MU	C5-C4-N3	-3.69	115.20	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CW	55	5MU	C5-C4-N3	-3.67	115.23	123.31
22	AV	54	5MU	C5-C4-N3	-3.54	115.52	123.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	GDP	AY	703	60	24,30,30	1.35	3 (12%)	31,47,47	2.00	8 (25%)
62	GDP	CY	703	60	24,30,30	1.39	3 (12%)	31,47,47	2.12	8 (25%)
61	FUA	AY	702	-	36,40,40	1.76	6 (16%)	46,64,64	1.51	5 (10%)
61	FUA	CY	702	-	36,40,40	1.78	6 (16%)	46,64,64	1.45	9 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GDP	AY	703	60	-	3/12/32/32	0/3/3/3
62	GDP	CY	703	60	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	FUA	AY	702	-	-	6/11/92/92	0/4/4/4
61	FUA	CY	702	-	-	6/11/92/92	0/4/4/4

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	702	FUA	C23-C22	-6.73	1.39	1.51
61	AY	702	FUA	C23-C22	-6.55	1.39	1.51
62	CY	703	GDP	C6-N1	4.45	1.40	1.33
61	AY	702	FUA	C23-C24	-4.27	1.39	1.53
61	CY	702	FUA	C23-C24	-4.26	1.39	1.53

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	CY	703	GDP	C2-N3-C4	5.62	121.78	115.36
62	AY	703	GDP	C2-N3-C4	5.36	121.48	115.36
62	CY	703	GDP	N3-C2-N1	-5.29	120.16	127.22
62	AY	703	GDP	N3-C2-N1	-5.29	120.17	127.22
61	AY	702	FUA	C13-C12-C11	-4.33	105.84	111.90

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

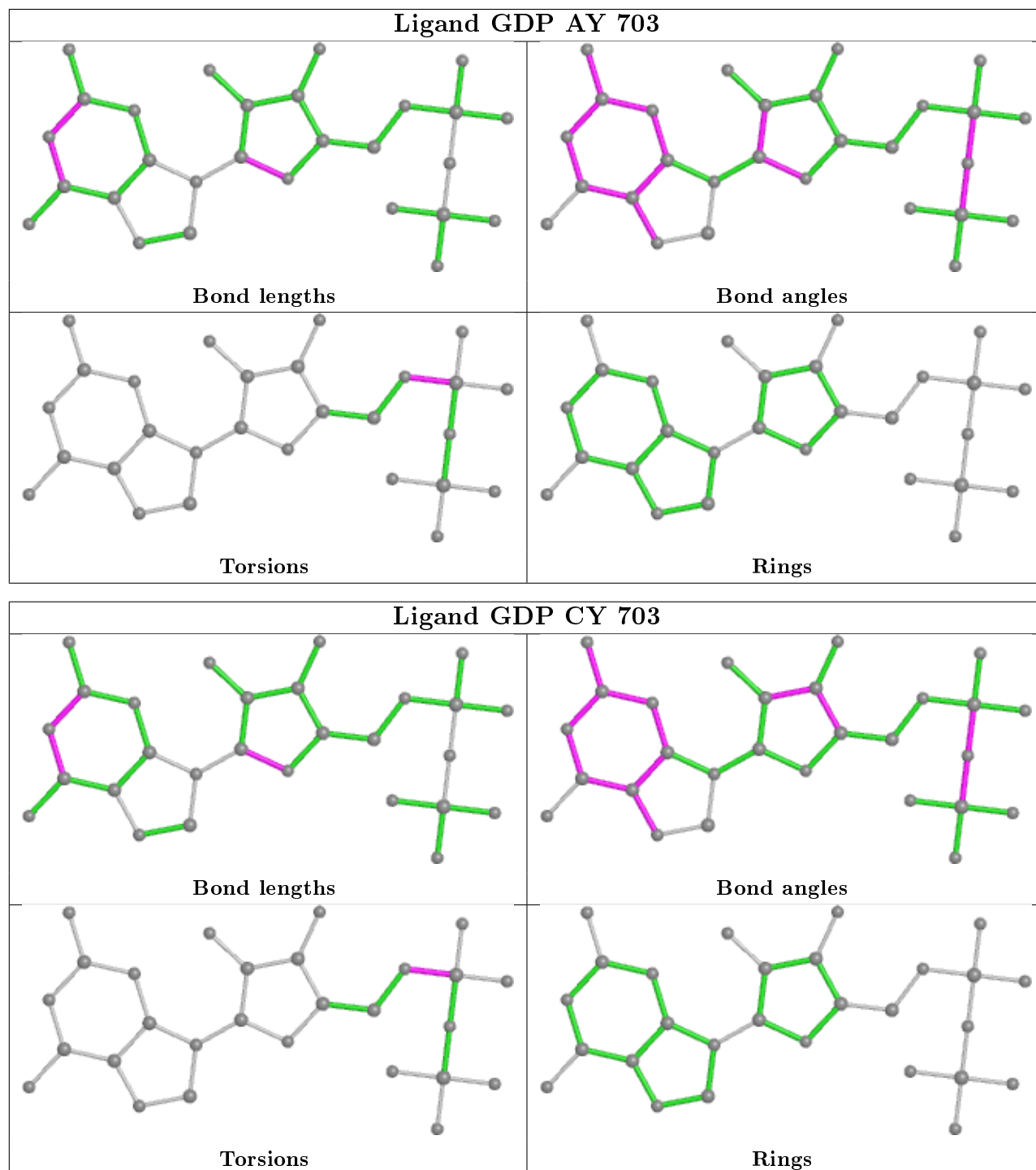
Mol	Chain	Res	Type	Atoms
61	AY	702	FUA	C13-C17-C22-C29
61	AY	702	FUA	C17-C22-C23-C24
61	AY	702	FUA	C29-C22-C23-C24
62	AY	703	GDP	C5'-O5'-PA-O3A
62	AY	703	GDP	C5'-O5'-PA-O1A

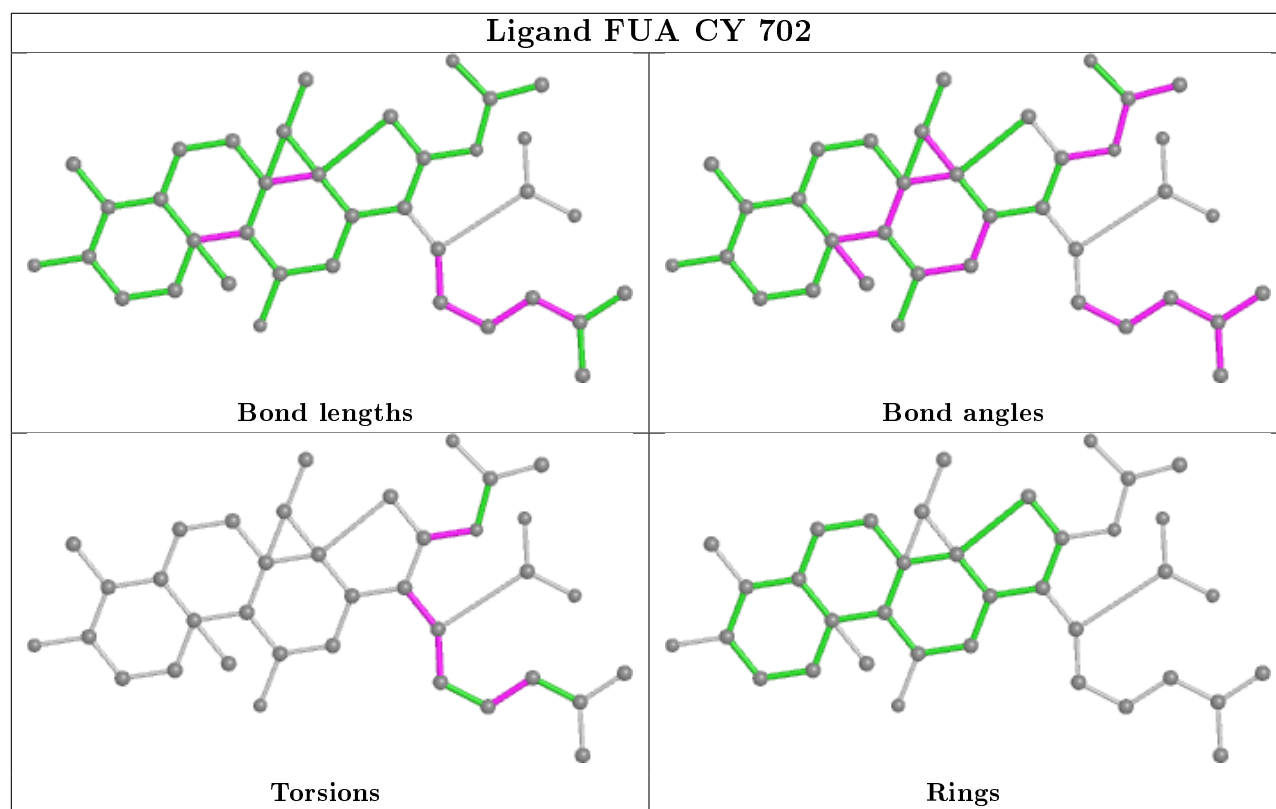
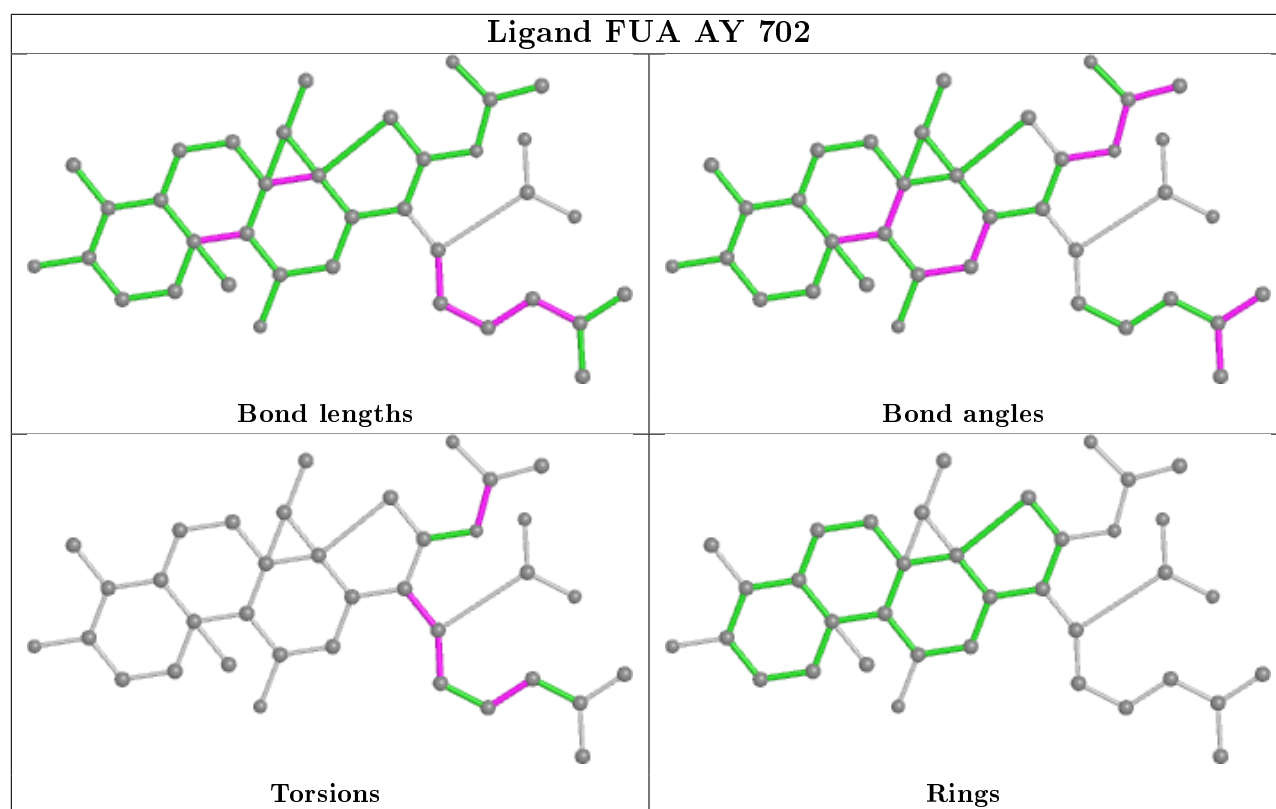
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	AI	2
9	CI	2
45	BL	1
41	DG	1
41	BG	1
45	DL	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DL	30:UNK	C	52:UNK	N	38.40
1	BL	30:UNK	C	52:UNK	N	36.36
1	BG	112:PRO	C	113:ARG	N	3.27
1	DG	112:PRO	C	113:ARG	N	3.05
1	CI	53:VAL	C	54:ASP	N	2.98

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.27	22 (1%) 73 60	23, 62, 148, 220	0
1	CA	1504/1522 (98%)	-0.51	15 (0%) 82 70	26, 65, 148, 220	0
2	AB	235/256 (91%)	-0.30	3 (1%) 77 63	40, 81, 147, 159	0
2	CB	235/256 (91%)	-0.32	1 (0%) 92 86	43, 82, 147, 158	0
3	AC	207/239 (86%)	-0.41	0 100 100	31, 72, 113, 118	0
3	CC	207/239 (86%)	-0.38	0 100 100	33, 75, 115, 121	0
4	AD	208/209 (99%)	-0.39	0 100 100	47, 79, 115, 124	0
4	CD	208/209 (99%)	-0.43	0 100 100	48, 80, 116, 125	0
5	AE	151/162 (93%)	-0.49	1 (0%) 87 78	25, 50, 90, 112	0
5	CE	151/162 (93%)	-0.46	1 (0%) 87 78	27, 52, 91, 112	0
6	AF	101/101 (100%)	-0.44	0 100 100	55, 85, 110, 118	0
6	CF	101/101 (100%)	-0.29	0 100 100	60, 87, 111, 118	0
7	AG	155/156 (99%)	-0.38	1 (0%) 89 81	51, 79, 109, 136	0
7	CG	155/156 (99%)	-0.39	2 (1%) 77 63	55, 81, 111, 136	0
8	AH	138/138 (100%)	-0.41	0 100 100	32, 54, 75, 82	0
8	CH	138/138 (100%)	-0.49	0 100 100	35, 56, 76, 83	0
9	AI	127/128 (99%)	-0.23	1 (0%) 86 75	50, 83, 114, 120	0
9	CI	127/128 (99%)	-0.36	1 (0%) 86 75	53, 86, 114, 120	0
10	AJ	99/105 (94%)	0.08	6 (6%) 21 12	47, 100, 155, 159	0
10	CJ	99/105 (94%)	0.18	3 (3%) 50 34	50, 102, 156, 159	0
11	AK	119/129 (92%)	-0.34	2 (1%) 70 55	42, 59, 100, 123	0
11	CK	119/129 (92%)	-0.28	1 (0%) 86 75	44, 60, 102, 124	0
12	AL	125/132 (94%)	-0.49	0 100 100	38, 57, 87, 127	0
12	CL	125/132 (94%)	-0.43	2 (1%) 72 57	39, 58, 88, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	-0.15	6 (4%) 30 19	68, 111, 139, 171	0
13	CM	125/126 (99%)	-0.16	8 (6%) 19 11	70, 112, 139, 172	0
14	AN	60/61 (98%)	-0.41	1 (1%) 70 55	39, 59, 92, 97	0
14	CN	60/61 (98%)	-0.42	0 100 100	44, 61, 93, 98	0
15	AO	88/89 (98%)	-0.57	0 100 100	35, 61, 91, 100	0
15	CO	88/89 (98%)	-0.54	0 100 100	38, 61, 94, 100	0
16	AP	84/88 (95%)	-0.45	0 100 100	54, 73, 96, 131	0
16	CP	84/88 (95%)	-0.43	1 (1%) 79 66	57, 74, 98, 132	0
17	AQ	100/105 (95%)	-0.56	0 100 100	43, 64, 89, 98	0
17	CQ	100/105 (95%)	-0.50	0 100 100	46, 66, 90, 97	0
18	AR	70/88 (79%)	-0.42	1 (1%) 75 61	42, 69, 94, 108	0
18	CR	70/88 (79%)	-0.51	1 (1%) 75 61	45, 70, 95, 109	0
19	AS	79/93 (84%)	-0.02	2 (2%) 57 41	77, 106, 144, 149	0
19	CS	79/93 (84%)	0.15	4 (5%) 28 17	78, 107, 144, 150	0
20	AT	99/106 (93%)	-0.37	0 100 100	63, 84, 126, 129	0
20	CT	99/106 (93%)	-0.37	0 100 100	64, 85, 127, 129	0
21	AU	25/27 (92%)	-0.24	0 100 100	63, 82, 118, 122	0
21	CU	25/27 (92%)	0.12	0 100 100	66, 86, 120, 123	0
22	AV	76/77 (98%)	-0.48	0 100 100	32, 67, 110, 127	0
22	AW	76/77 (98%)	-0.43	1 (1%) 77 63	71, 168, 192, 201	0
22	CV	76/77 (98%)	-0.61	0 100 100	47, 84, 121, 151	0
22	CW	76/77 (98%)	-0.37	1 (1%) 77 63	78, 176, 200, 210	0
23	AX	11/25 (44%)	0.09	0 100 100	28, 94, 149, 166	0
23	CX	11/25 (44%)	0.01	0 100 100	45, 106, 156, 168	0
24	AY	667/691 (96%)	-0.17	9 (1%) 77 63	61, 99, 140, 150	0
24	CY	667/691 (96%)	0.08	23 (3%) 45 30	73, 108, 148, 161	0
25	B0	84/85 (98%)	0.05	6 (7%) 16 9	67, 82, 140, 163	0
25	D0	84/85 (98%)	0.37	9 (10%) 6 3	69, 84, 141, 163	0
26	B1	94/98 (95%)	-0.46	1 (1%) 80 68	41, 70, 118, 128	0
26	D1	94/98 (95%)	-0.34	0 100 100	53, 80, 123, 131	0
27	B2	71/72 (98%)	-0.30	2 (2%) 53 37	77, 116, 150, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	-0.15	2 (2%) 53 37	95, 119, 146, 163	0
28	B3	60/60 (100%)	-0.08	1 (1%) 70 55	63, 88, 114, 135	0
28	D3	60/60 (100%)	-0.02	2 (3%) 46 31	64, 89, 114, 134	0
29	B4	58/71 (81%)	0.07	3 (5%) 27 17	76, 135, 220, 222	0
29	D4	58/71 (81%)	0.27	7 (12%) 4 3	77, 137, 220, 222	0
30	B5	59/60 (98%)	-0.08	3 (5%) 28 17	52, 80, 153, 172	0
30	D5	59/60 (98%)	-0.03	4 (6%) 17 10	52, 80, 153, 172	0
31	B6	50/54 (92%)	0.00	2 (4%) 38 25	56, 89, 107, 117	0
31	D6	50/54 (92%)	-0.26	1 (2%) 65 49	56, 90, 108, 117	0
32	B7	49/49 (100%)	-0.34	2 (4%) 37 24	47, 64, 119, 132	0
32	D7	49/49 (100%)	-0.39	0 100 100	47, 64, 120, 132	0
33	B8	64/65 (98%)	-0.37	1 (1%) 72 57	63, 75, 105, 125	0
33	D8	64/65 (98%)	-0.26	1 (1%) 72 57	65, 76, 105, 126	0
34	B9	37/37 (100%)	-0.43	0 100 100	60, 71, 85, 89	0
34	D9	37/37 (100%)	-0.30	1 (2%) 54 38	60, 73, 87, 91	0
35	BA	2901/2915 (99%)	-0.39	27 (0%) 84 73	30, 76, 162, 221	0
35	DA	2901/2915 (99%)	-0.52	32 (1%) 80 68	29, 77, 162, 221	0
36	BB	119/122 (97%)	-0.54	0 100 100	65, 106, 138, 183	0
36	DB	119/122 (97%)	-0.72	0 100 100	66, 108, 138, 183	0
37	BC	228/229 (99%)	-0.13	4 (1%) 68 53	42, 97, 147, 160	0
37	DC	228/229 (99%)	0.09	12 (5%) 26 16	43, 98, 148, 162	0
38	BD	275/276 (99%)	-0.52	0 100 100	31, 52, 82, 101	0
38	DD	275/276 (99%)	-0.51	1 (0%) 92 86	32, 52, 82, 101	0
39	BE	205/206 (99%)	-0.33	4 (1%) 65 49	44, 77, 128, 135	0
39	DE	205/206 (99%)	-0.29	3 (1%) 73 60	44, 77, 128, 134	0
40	BF	208/210 (99%)	0.01	10 (4%) 30 19	53, 110, 166, 177	0
40	DF	208/210 (99%)	-0.01	11 (5%) 26 16	53, 111, 166, 176	0
41	BG	181/182 (99%)	-0.27	4 (2%) 62 45	63, 95, 131, 143	0
41	DG	181/182 (99%)	-0.03	6 (3%) 46 31	86, 110, 137, 151	0
42	BH	167/180 (92%)	0.06	6 (3%) 42 28	81, 117, 143, 159	0
42	DH	167/180 (92%)	0.04	4 (2%) 59 42	81, 118, 143, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BJ	0/173	-	-	-	-
43	DJ	0/173	-	-	-	-
44	BK	140/147 (95%)	1.96	61 (43%) 0 0	162, 180, 186, 188	0
44	DK	140/147 (95%)	1.68	49 (35%) 0 0	162, 180, 186, 187	0
45	BL	0/125	-	-	-	-
45	BM	0/125	-	-	-	-
45	Bl	0/125	-	-	-	-
45	Bm	0/125	-	-	-	-
45	DL	0/125	-	-	-	-
45	DM	0/125	-	-	-	-
45	Dl	0/125	-	-	-	-
45	Dm	0/125	-	-	-	-
46	BN	139/140 (99%)	-0.30	2 (1%) 75 61	60, 91, 132, 137	0
46	DN	139/140 (99%)	-0.25	1 (0%) 87 78	61, 91, 132, 137	0
47	BO	122/122 (100%)	-0.45	0 100 100	35, 60, 73, 86	0
47	DO	122/122 (100%)	-0.43	0 100 100	36, 61, 73, 88	0
48	BP	146/150 (97%)	0.02	4 (2%) 54 38	46, 111, 137, 157	0
48	DP	146/150 (97%)	0.10	4 (2%) 54 38	50, 113, 137, 157	0
49	BQ	141/141 (100%)	-0.38	0 100 100	45, 65, 88, 119	0
49	DQ	141/141 (100%)	-0.41	0 100 100	45, 66, 89, 120	0
50	BR	117/118 (99%)	-0.37	1 (0%) 84 73	49, 81, 101, 128	0
50	DR	117/118 (99%)	-0.28	1 (0%) 84 73	53, 82, 101, 128	0
51	BS	99/112 (88%)	-0.19	2 (2%) 65 49	82, 116, 140, 144	0
51	DS	99/112 (88%)	0.28	5 (5%) 28 17	83, 117, 141, 145	0
52	BT	138/146 (94%)	-0.13	4 (2%) 51 35	55, 83, 149, 176	0
52	DT	138/146 (94%)	-0.18	5 (3%) 42 28	57, 84, 149, 177	0
53	BU	117/118 (99%)	-0.36	0 100 100	62, 80, 114, 135	0
53	DU	117/118 (99%)	-0.36	0 100 100	62, 81, 115, 134	0
54	BV	101/101 (100%)	-0.02	1 (0%) 82 70	59, 116, 133, 141	0
54	DV	101/101 (100%)	0.18	6 (5%) 22 13	61, 116, 134, 140	0
55	BW	113/113 (100%)	-0.28	0 100 100	61, 79, 119, 158	0
55	DW	113/113 (100%)	-0.16	0 100 100	63, 80, 120, 159	0
56	BX	93/96 (96%)	-0.18	0 100 100	76, 91, 110, 114	0
56	DX	93/96 (96%)	-0.22	0 100 100	76, 92, 111, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
57	BY	107/110 (97%)	0.08	2 (1%) 66 51	78, 127, 149, 155	0
57	DY	107/110 (97%)	0.41	4 (3%) 41 27	78, 127, 149, 155	0
58	BZ	185/206 (89%)	-0.23	1 (0%) 91 83	47, 90, 135, 143	0
58	DZ	185/206 (89%)	-0.09	1 (0%) 91 83	68, 99, 138, 146	0
All	All	22794/24788 (91%)	-0.29	446 (1%) 65 49	23, 82, 155, 222	0

The worst 5 of 446 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BA	654(K)	C	14.8
1	CA	1036	G	13.4
52	BT	138	ALA	13.1
35	DA	654(D)	G	13.0
35	BA	654(F)	C	11.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	5MU	CW	55	20/22	0.81	0.13	178,179,186,186	0
22	5MU	AW	55	20/22	0.82	0.14	161,165,168,168	0
22	5MU	AV	54	20/22	0.95	0.13	82,84,86,86	0
22	5MU	CV	54	20/22	0.97	0.11	89,92,95,96	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

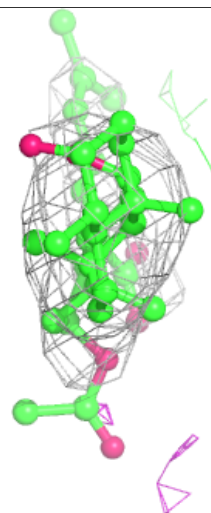
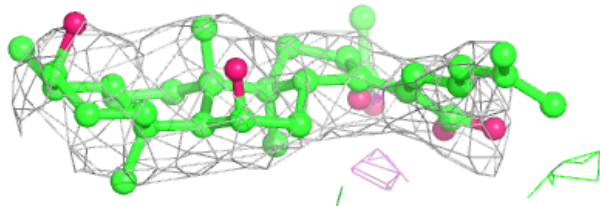
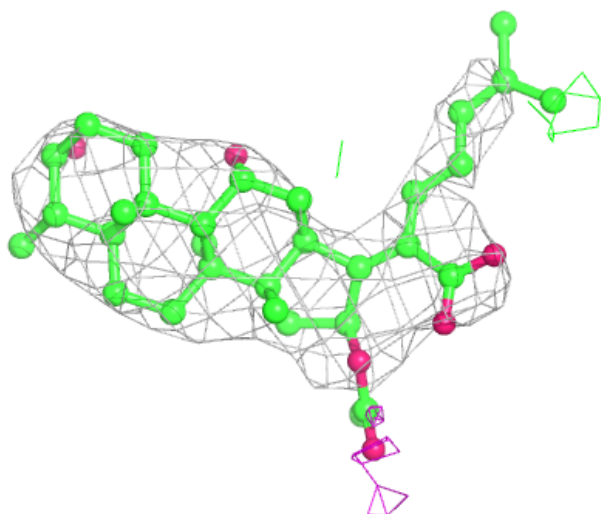
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	FUA	AY	702	37/37	0.90	0.43	98,102,110,111	0
61	FUA	CY	702	37/37	0.90	0.35	102,104,107,109	0
59	ZN	D4	101	1/1	0.90	0.07	164,164,164,164	0
59	ZN	B4	101	1/1	0.91	0.12	122,122,122,122	0
62	GDP	CY	703	28/28	0.95	0.15	81,87,94,95	0
62	GDP	AY	703	28/28	0.96	0.17	78,82,83,84	0
60	MG	AY	701	1/1	0.98	0.22	30,30,30,30	0
59	ZN	CD	301	1/1	0.99	0.28	49,49,49,49	0
60	MG	CY	701	1/1	0.99	0.12	39,39,39,39	0
59	ZN	B9	101	1/1	0.99	0.15	62,62,62,62	0
59	ZN	CN	101	1/1	1.00	0.16	66,66,66,66	0
59	ZN	AD	301	1/1	1.00	0.28	32,32,32,32	0
59	ZN	AN	101	1/1	1.00	0.16	35,35,35,35	0
59	ZN	D9	101	1/1	1.00	0.12	86,86,86,86	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

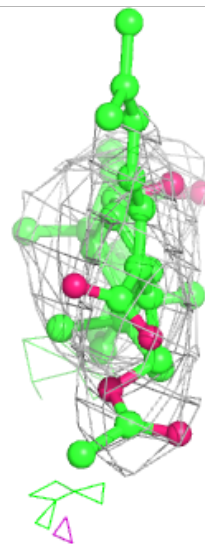
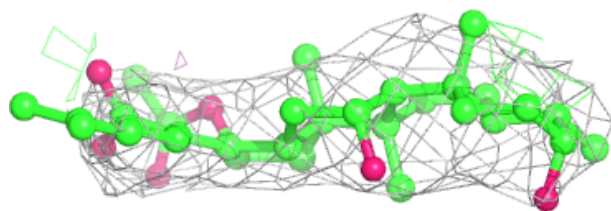
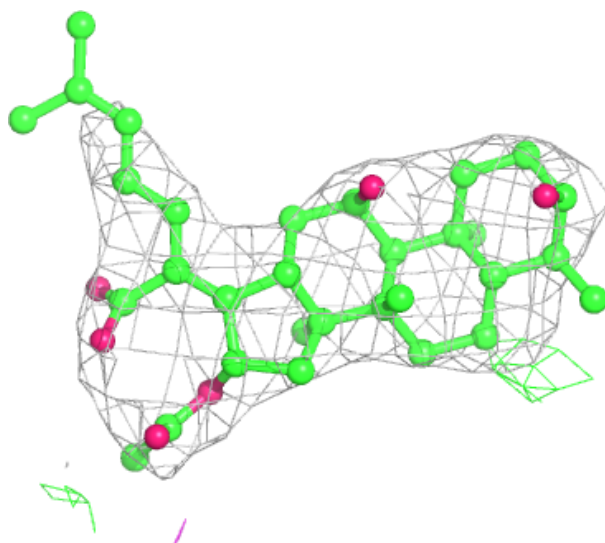
Electron density around FUA AY 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



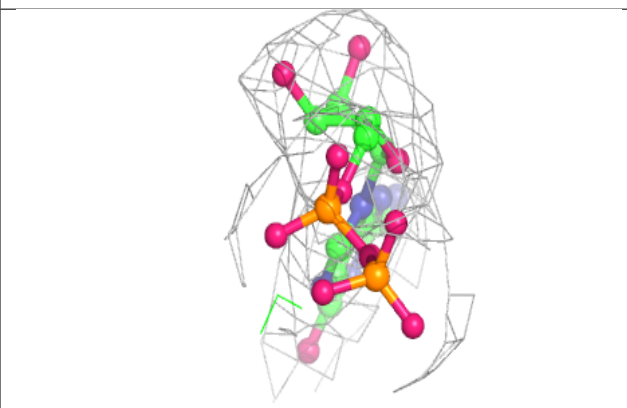
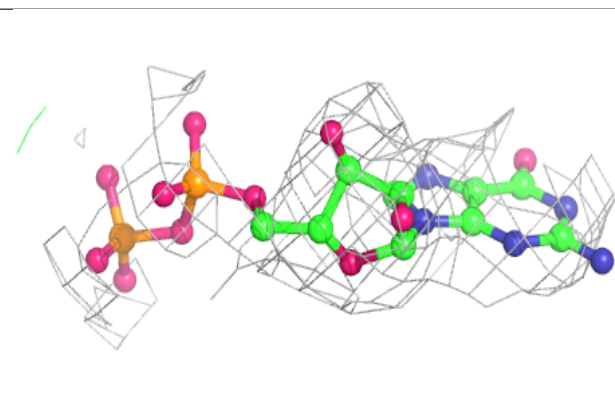
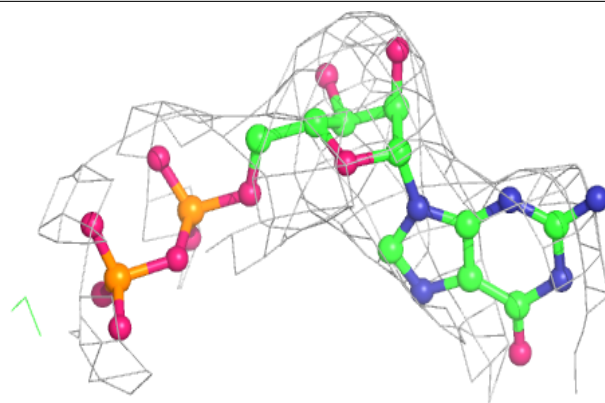
Electron density around FUA CY 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

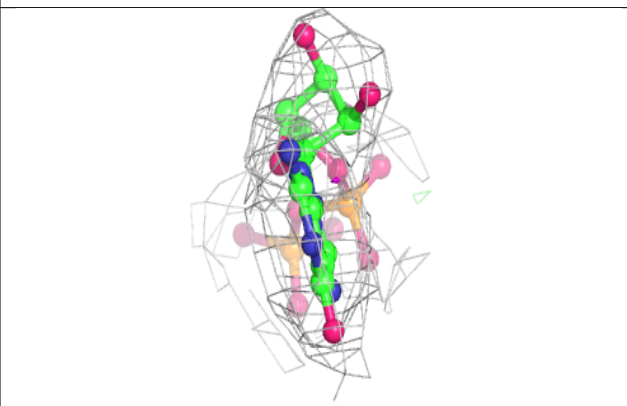
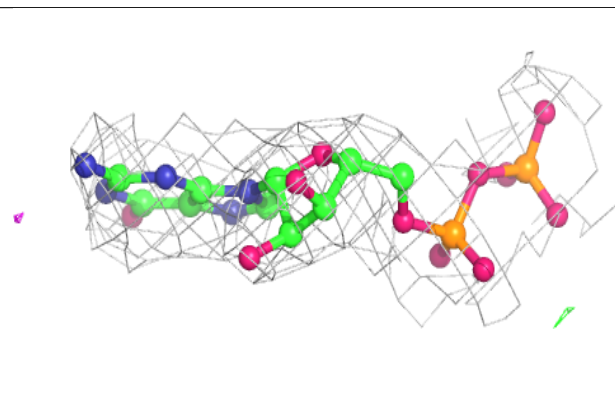
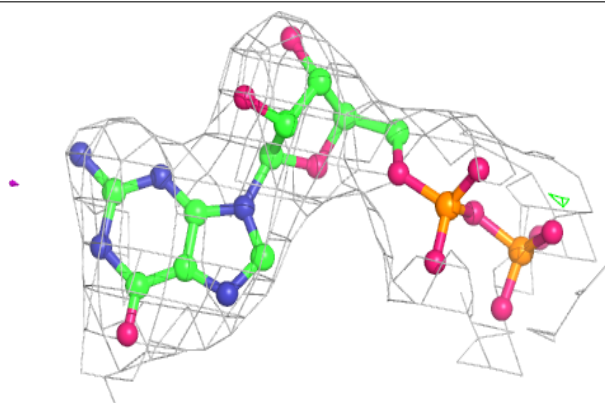


Electron density around GDP CY 703:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GDP AY 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.